



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:26 PM UTC

PDB ID : 9CQK / pdb_00009cqk
Title : Horse liver alcohol dehydrogenase F93W in complex with NADH and N-cylcohexyl formamide
Authors : Mukherjee, S.; Boxer, S.G.
Deposited on : 2024-07-19
Resolution : 1.65 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

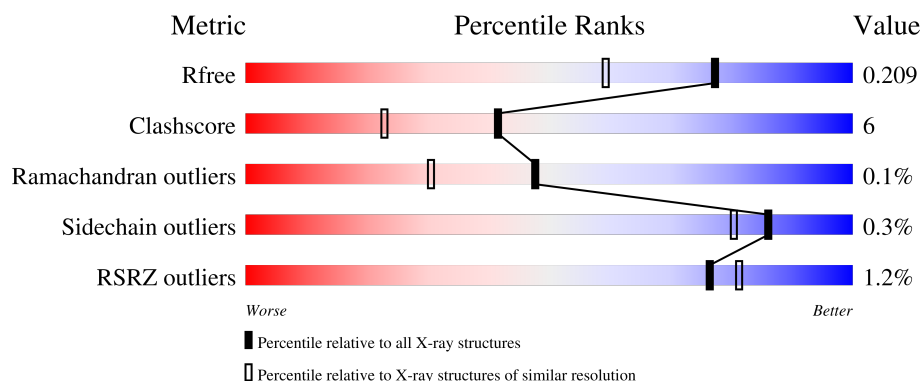
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>36%</div> <div>..</div> </div> </div>
1	B	377	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>41%</div> <div>..</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6248 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
			2788	1771	473	521	23			
1	B	374	Total	C	N	O	S	0	2	0
			2797	1777	474	523	23			

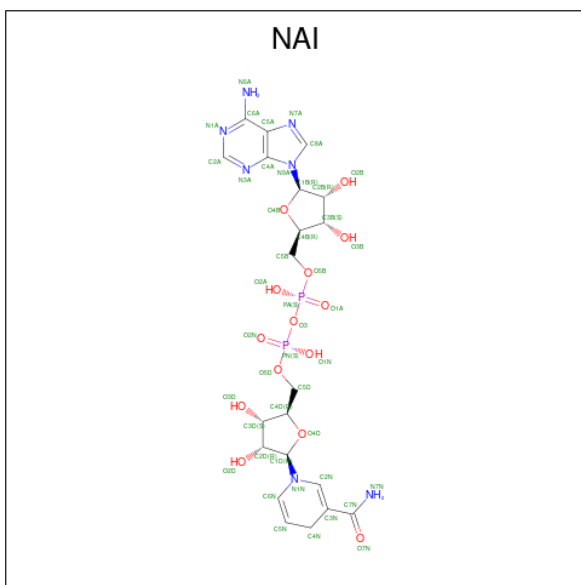
There are 8 discrepancies between the modelled and reference sequences:

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
A	93	TRP	PHE	engineered mutation	UNP P00327
B	-2	GLY	-	expression tag	UNP P00327
B	-1	ALA	-	expression tag	UNP P00327
B	0	GLY	-	expression tag	UNP P00327
B	93	TRP	PHE	engineered mutation	UNP P00327

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

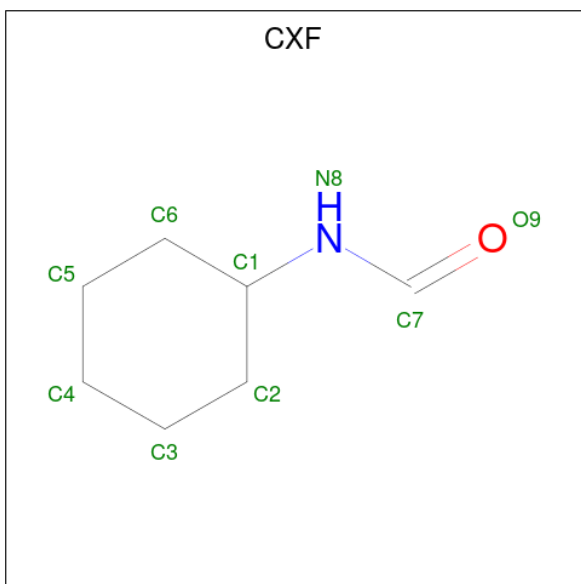
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is CYCLOHEXYLFORMAMIDE (CCD ID: CXF) (formula: $C_7H_{13}NO$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

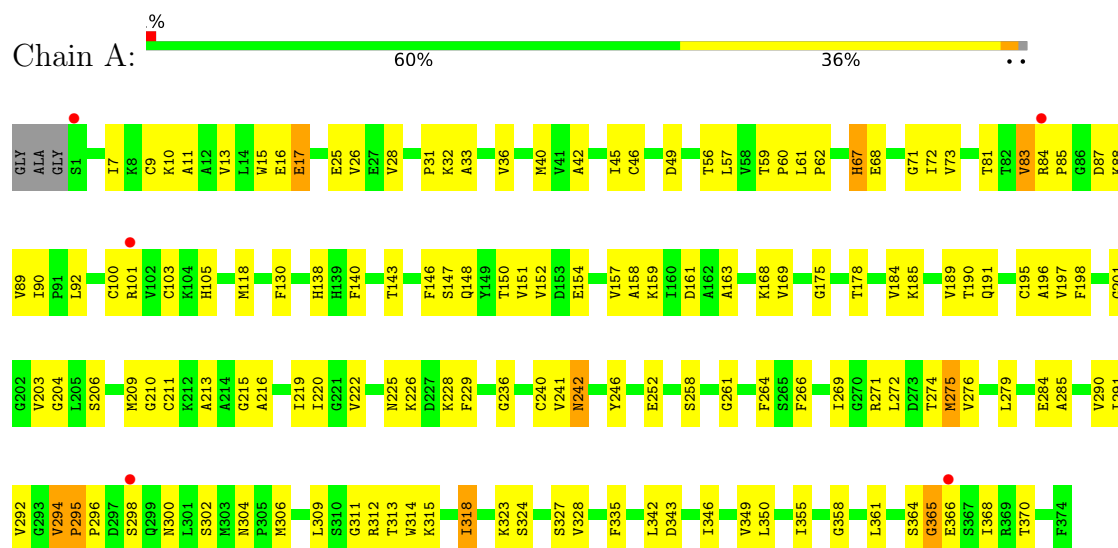
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	308	Total	O	0	0
			308	308		
5	B	245	Total	O	0	0
			245	245		

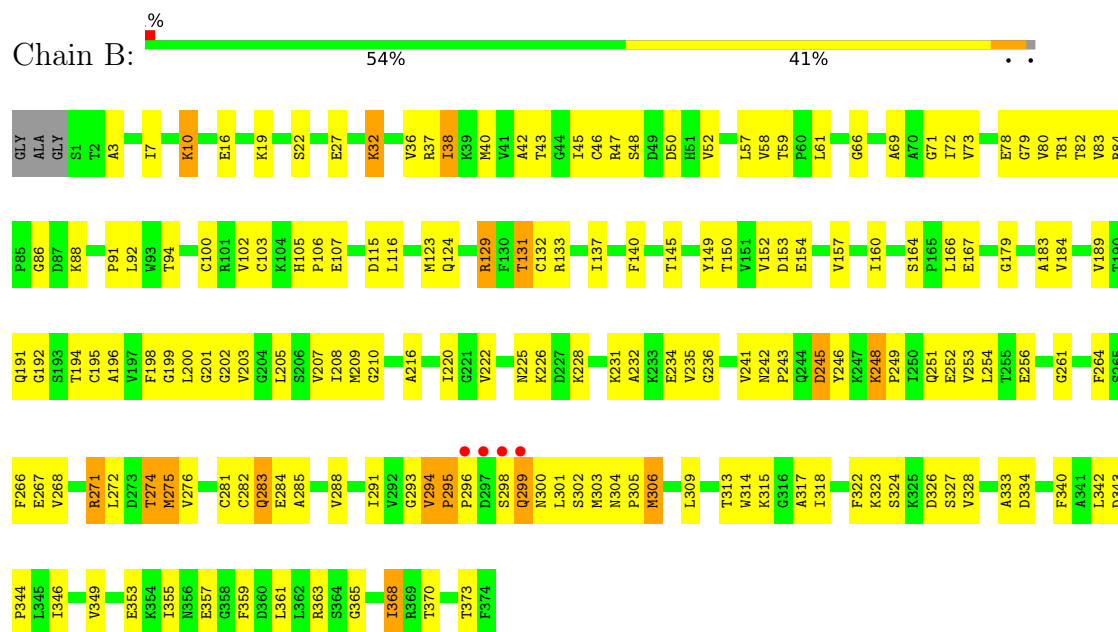
3 Residue-property plots

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	42.57Å 45.45Å 92.14Å 75.85° 78.69° 77.26°	Depositor
Resolution (Å)	36.03 – 1.65 36.03 – 1.65	Depositor EDS
% Data completeness (in resolution range)	88.7 (36.03-1.65) 88.7 (36.03-1.65)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.65Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.196 , 0.209 0.196 , 0.209	Depositor DCC
R_{free} test set	3476 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.7	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	0.95	EDS
Total number of atoms	6248	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 7.04% 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: ZN, NAI, CXF

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	2.01	114/2841 (4.0%)	1.08	8/3841 (0.2%)
1	B	2.08	142/2856 (5.0%)	1.19	18/3861 (0.5%)
All	All	2.04	256/5697 (4.5%)	1.14	26/7702 (0.3%)

All (256) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	ALA	C-O	-10.69	1.11	1.24
1	B	94	THR	C-O	-8.95	1.14	1.24
1	B	208	ILE	C-O	-8.93	1.13	1.24
1	B	36	VAL	C-O	-8.89	1.14	1.24
1	B	84	ARG	C-O	-8.82	1.16	1.24
1	B	295	PRO	C-O	-8.67	1.14	1.24
1	A	328	VAL	C-O	-8.47	1.17	1.24
1	A	197	VAL	C-O	-8.23	1.15	1.24
1	A	346	ILE	C-O	-8.17	1.15	1.24
1	B	205	LEU	C-O	-7.90	1.14	1.24
1	A	241	VAL	C-O	-7.81	1.16	1.24
1	B	59	THR	C-O	-7.74	1.15	1.24
1	A	264	PHE	C-O	-7.72	1.15	1.23
1	A	89	VAL	C-O	-7.64	1.15	1.23
1	B	253	VAL	C-O	-7.63	1.15	1.24
1	B	102	VAL	C-O	-7.58	1.15	1.24
1	A	258	SER	C-O	-7.58	1.14	1.24
1	A	140	PHE	C-O	-7.53	1.15	1.24
1	A	33	ALA	C-O	-7.52	1.15	1.23
1	B	203	VAL	C-O	-7.49	1.14	1.24
1	A	294	VAL	C-O	-7.46	1.15	1.24
1	B	306	MET	C-O	-7.43	1.14	1.24
1	B	79	GLY	C-O	-7.35	1.14	1.24
1	A	92	LEU	C-O	-7.32	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	ILE	C-O	-7.32	1.15	1.24
1	B	275	MET	C-O	-7.29	1.15	1.24
1	A	13	VAL	C-O	-7.27	1.16	1.24
1	A	28	VAL	C-O	-7.26	1.16	1.24
1	A	216	ALA	C-O	-7.24	1.15	1.23
1	A	151	VAL	C-O	-7.20	1.16	1.24
1	A	266	PHE	C-O	-7.16	1.16	1.23
1	B	46	CYS	C-O	-7.10	1.15	1.23
1	A	178	THR	C-O	-7.08	1.16	1.24
1	A	32	LYS	C-O	-7.00	1.15	1.23
1	A	304	ASN	C-O	-7.00	1.15	1.24
1	A	150	THR	C-O	-6.99	1.15	1.23
1	B	302[A]	SER	CA-C	6.98	1.61	1.52
1	B	302[B]	SER	CA-C	6.98	1.61	1.52
1	A	292	VAL	C-O	-6.97	1.15	1.24
1	B	80	VAL	C-O	-6.94	1.15	1.24
1	B	282	CYS	C-O	-6.94	1.15	1.23
1	B	92	LEU	C-O	-6.92	1.16	1.24
1	B	232	ALA	C-O	-6.91	1.16	1.24
1	B	198	PHE	C-O	-6.89	1.15	1.24
1	B	22	SER	C-O	-6.89	1.15	1.24
1	B	318	ILE	C-O	-6.89	1.16	1.24
1	B	88	LYS	C-O	-6.88	1.15	1.23
1	A	60	PRO	C-O	-6.87	1.15	1.23
1	B	71	GLY	C-O	-6.86	1.16	1.23
1	A	36	VAL	C-O	-6.84	1.17	1.24
1	A	220	ILE	C-O	-6.84	1.16	1.24
1	A	295	PRO	C-O	-6.83	1.16	1.24
1	B	78	GLU	C-O	-6.82	1.15	1.23
1	B	248	LYS	C-O	-6.82	1.18	1.24
1	A	7	ILE	C-O	-6.81	1.16	1.24
1	B	137	ILE	C-O	-6.79	1.17	1.24
1	A	313	THR	C-O	-6.77	1.15	1.24
1	A	42	ALA	C-O	-6.73	1.15	1.23
1	A	45	ILE	C-O	-6.73	1.16	1.24
1	A	71	GLY	C-O	-6.73	1.17	1.23
1	B	373	THR	C-O	-6.70	1.16	1.24
1	A	291	ILE	C-O	-6.66	1.16	1.24
1	A	143	THR	C-O	-6.66	1.15	1.24
1	B	38	ILE	C-O	-6.65	1.17	1.24
1	B	274	THR	C-O	-6.65	1.15	1.24
1	B	245	ASP	C-O	-6.62	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	THR	C-O	-6.60	1.16	1.23
1	B	252	GLU	C-O	-6.60	1.16	1.24
1	A	163	ALA	C-O	-6.59	1.15	1.24
1	A	190	THR	C-O	-6.55	1.15	1.23
1	B	368	ILE	C-O	-6.55	1.16	1.24
1	B	202	GLY	C-O	-6.54	1.16	1.23
1	B	210	GLY	C-O	-6.53	1.16	1.23
1	A	229	PHE	C-O	-6.51	1.16	1.24
1	B	45	ILE	C-O	-6.51	1.16	1.24
1	A	157	VAL	C-O	-6.50	1.16	1.23
1	A	318	ILE	C-O	-6.46	1.16	1.24
1	A	90	ILE	C-O	-6.45	1.17	1.23
1	B	303	MET	C-O	-6.45	1.16	1.23
1	B	251	GLN	C-O	-6.44	1.16	1.24
1	A	279	LEU	C-O	-6.43	1.16	1.24
1	B	152	VAL	C-O	-6.43	1.17	1.23
1	A	355	ILE	C-O	-6.41	1.16	1.24
1	B	300	ASN	C-O	-6.39	1.15	1.23
1	A	130	PHE	C-O	-6.34	1.15	1.24
1	A	276	VAL	C-O	-6.34	1.16	1.24
1	B	7	ILE	C-O	-6.31	1.17	1.24
1	B	69	ALA	C-O	-6.31	1.16	1.23
1	B	157	VAL	C-O	-6.31	1.16	1.23
1	B	191	GLN	C-O	-6.29	1.16	1.23
1	A	252	GLU	C-O	-6.27	1.16	1.24
1	A	195	CYS	C-O	-6.27	1.15	1.23
1	A	242	ASN	C-O	-6.25	1.17	1.24
1	A	222	VAL	C-O	-6.25	1.17	1.24
1	A	211	CYS	C-O	-6.24	1.16	1.24
1	B	133	ARG	C-O	-6.21	1.15	1.23
1	B	294	VAL	C-O	-6.19	1.17	1.24
1	B	334	ASP	C-O	-6.19	1.16	1.24
1	B	153	ASP	C-O	-6.18	1.16	1.23
1	B	72	ILE	C-O	-6.16	1.17	1.24
1	A	309	LEU	C-O	-6.14	1.16	1.24
1	A	300	ASN	C-O	-6.13	1.16	1.23
1	B	58	VAL	C-O	-6.12	1.17	1.24
1	B	201	GLY	C-O	-6.12	1.17	1.23
1	B	216	ALA	C-O	-6.12	1.16	1.23
1	A	198	PHE	C-O	-6.11	1.16	1.24
1	A	312	ARG	C-O	-6.11	1.16	1.23
1	A	225	ASN	C-O	-6.10	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	LEU	C-O	-6.08	1.17	1.24
1	A	67	HIS	C-O	-6.06	1.16	1.23
1	B	322	PHE	C-O	-6.04	1.16	1.24
1	B	166	LEU	C-O	-6.03	1.16	1.24
1	B	195	CYS	C-O	-6.01	1.16	1.23
1	A	361	LEU	C-O	-6.01	1.17	1.24
1	A	275	MET	C-O	-6.00	1.17	1.24
1	A	100	CYS	C-O	-5.99	1.15	1.23
1	A	31	PRO	C-O	-5.97	1.17	1.23
1	A	184	VAL	C-O	-5.97	1.16	1.24
1	B	355	ILE	C-O	-5.96	1.17	1.24
1	B	234	GLU	C-O	-5.95	1.16	1.24
1	B	42	ALA	C-O	-5.95	1.16	1.23
1	A	343	ASP	C-O	-5.94	1.18	1.24
1	B	231	LYS	C-O	-5.94	1.17	1.24
1	B	131	THR	C-O	-5.93	1.16	1.23
1	A	315	LYS	C-O	-5.93	1.16	1.23
1	A	25	GLU	C-O	-5.92	1.16	1.24
1	A	311	GLY	C-O	-5.92	1.16	1.23
1	B	32	LYS	C-O	-5.92	1.17	1.23
1	B	140	PHE	C-O	-5.90	1.17	1.24
1	B	304	ASN	C-O	-5.90	1.16	1.24
1	A	46	CYS	C-O	-5.88	1.17	1.23
1	A	335	PHE	C-O	-5.87	1.17	1.24
1	B	222	VAL	C-O	-5.87	1.17	1.24
1	A	118	MET	C-O	-5.85	1.17	1.24
1	B	346	ILE	C-O	-5.82	1.17	1.24
1	B	194	THR	C-O	-5.81	1.17	1.24
1	B	254	LEU	C-O	-5.81	1.17	1.24
1	A	169	VAL	C-O	-5.80	1.15	1.24
1	B	276	VAL	C-O	-5.80	1.17	1.24
1	B	328	VAL	C-O	-5.80	1.19	1.24
1	A	314	TRP	C-O	-5.80	1.17	1.24
1	A	206	SER	C-O	-5.79	1.17	1.24
1	B	283	GLN	C-O	-5.79	1.16	1.23
1	B	267	GLU	C-O	-5.78	1.17	1.24
1	B	220	ILE	C-O	-5.76	1.18	1.24
1	B	266	PHE	C-O	-5.75	1.17	1.23
1	A	201	GLY	C-O	-5.75	1.18	1.23
1	B	241	VAL	C-O	-5.74	1.18	1.24
1	A	240	CYS	C-O	-5.73	1.17	1.23
1	A	87	ASP	C-O	-5.72	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	THR	C-O	-5.72	1.18	1.24
1	B	189	VAL	C-O	-5.71	1.17	1.24
1	B	225	ASN	C-O	-5.71	1.17	1.24
1	A	210	GLY	C-O	-5.70	1.17	1.23
1	A	213	ALA	C-O	-5.70	1.17	1.24
1	B	47	ARG	C-O	-5.69	1.17	1.24
1	B	73	VAL	C-O	-5.69	1.18	1.24
1	B	305	PRO	C-O	-5.68	1.16	1.24
1	A	203	VAL	C-O	-5.68	1.17	1.24
1	B	91	PRO	C-O	-5.67	1.17	1.23
1	B	192	GLY	C-O	-5.66	1.16	1.24
1	A	11	ALA	C-O	-5.65	1.17	1.23
1	B	323	LYS	C-O	-5.64	1.17	1.24
1	A	358	GLY	C-O	-5.64	1.17	1.23
1	A	105	HIS	C-O	-5.63	1.16	1.23
1	B	83	VAL	C-O	-5.63	1.17	1.23
1	B	82	THR	C-O	-5.61	1.16	1.24
1	B	150	THR	C-O	-5.60	1.16	1.23
1	A	57	LEU	C-O	-5.58	1.17	1.24
1	A	272	LEU	C-O	-5.58	1.17	1.24
1	A	61	LEU	C-O	-5.56	1.18	1.24
1	A	290	VAL	C-O	-5.55	1.18	1.24
1	A	16	GLU	C-O	-5.55	1.17	1.23
1	B	200	LEU	C-O	-5.55	1.16	1.23
1	A	83	VAL	C-O	-5.54	1.17	1.23
1	B	285	ALA	C-O	-5.51	1.16	1.24
1	B	196	ALA	C-O	-5.49	1.17	1.24
1	B	207	VAL	C-O	-5.49	1.17	1.24
1	A	152	VAL	C-O	-5.49	1.18	1.24
1	B	333	ALA	C-O	-5.48	1.17	1.24
1	B	342	LEU	C-O	-5.47	1.16	1.23
1	A	68	GLU	C-O	-5.46	1.17	1.24
1	B	81	THR	C-O	-5.46	1.17	1.24
1	A	85	PRO	C-O	-5.46	1.17	1.23
1	B	235	VAL	C-O	-5.46	1.18	1.24
1	A	72	ILE	C-O	-5.46	1.18	1.24
1	B	124	GLN	C-O	-5.45	1.17	1.24
1	B	243	PRO	C-O	-5.42	1.17	1.24
1	A	342	LEU	C-O	-5.42	1.16	1.23
1	B	10	LYS	C-O	-5.40	1.17	1.23
1	A	26	VAL	C-O	-5.39	1.18	1.23
1	B	317	ALA	C-O	-5.39	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	CYS	C-O	-5.38	1.16	1.24
1	A	159	LYS	C-O	-5.37	1.17	1.23
1	A	161	ASP	C-O	-5.37	1.17	1.24
1	B	271	ARG	C-O	-5.37	1.17	1.23
1	A	168	LYS	C-O	-5.36	1.16	1.23
1	A	365	GLY	C-O	-5.35	1.17	1.24
1	B	57	LEU	C-O	-5.35	1.18	1.24
1	B	183	ALA	C-O	-5.33	1.17	1.24
1	B	179	GLY	C-O	-5.31	1.17	1.23
1	B	132	CYS	C-O	-5.31	1.17	1.23
1	B	37	ARG	C-O	-5.27	1.17	1.24
1	B	272	LEU	C-O	-5.27	1.18	1.24
1	B	106	PRO	C-O	-5.26	1.18	1.24
1	A	236	GLY	C-O	-5.26	1.16	1.23
1	B	291	ILE	C-O	-5.23	1.17	1.24
1	B	48	SER	C-O	-5.23	1.17	1.24
1	B	164	SER	C-O	-5.23	1.17	1.24
1	B	340	PHE	C-O	-5.23	1.17	1.23
1	B	370	THR	C-O	-5.23	1.17	1.24
1	A	88	LYS	C-O	-5.22	1.17	1.24
1	B	86	GLY	C-O	-5.22	1.16	1.24
1	B	313	THR	C-O	-5.22	1.17	1.24
1	A	189	VAL	C-O	-5.22	1.18	1.24
1	B	236	GLY	C-O	-5.21	1.16	1.23
1	A	302	SER	C-O	-5.21	1.17	1.24
1	B	184	VAL	C-O	-5.21	1.18	1.24
1	B	129	ARG	C-O	-5.20	1.16	1.23
1	A	73	VAL	C-O	-5.20	1.18	1.24
1	B	349	VAL	C-O	-5.20	1.18	1.24
1	A	219	ILE	C-O	-5.19	1.18	1.24
1	B	145	THR	C-O	-5.18	1.17	1.24
1	A	147	SER	C-O	-5.18	1.17	1.23
1	B	293	GLY	C-O	-5.18	1.16	1.23
1	A	49	ASP	C-O	-5.17	1.18	1.24
1	B	264	PHE	C-O	-5.17	1.18	1.23
1	B	52	VAL	C-O	-5.16	1.18	1.24
1	A	285	ALA	C-O	-5.16	1.17	1.24
1	B	100	CYS	C-O	-5.15	1.16	1.23
1	B	103	CYS	C-O	-5.14	1.17	1.24
1	B	261	GLY	C-O	-5.14	1.17	1.23
1	B	3	ALA	C-O	-5.13	1.17	1.23
1	A	146	PHE	C-O	-5.13	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	CYS	C-O	-5.13	1.17	1.23
1	B	314	TRP	C-O	-5.12	1.18	1.24
1	B	199	GLY	C-O	-5.12	1.17	1.23
1	B	154	GLU	C-O	-5.12	1.18	1.24
1	B	361	LEU	C-O	-5.11	1.17	1.24
1	A	158	ALA	C-O	-5.10	1.18	1.24
1	B	353	GLU	C-O	-5.09	1.17	1.24
1	A	154	GLU	C-O	-5.09	1.17	1.24
1	B	149	TYR	C-O	-5.09	1.17	1.23
1	A	261	GLY	C-O	-5.07	1.17	1.23
1	B	209	MET	C-O	-5.07	1.18	1.24
1	B	160	ILE	C-O	-5.06	1.17	1.23
1	B	66	GLY	C-O	-5.06	1.17	1.23
1	B	315	LYS	C-O	-5.05	1.17	1.23
1	B	256	GLU	C-O	-5.05	1.18	1.24
1	A	228	LYS	C-O	-5.03	1.17	1.24
1	A	138	HIS	C-O	-5.02	1.17	1.23
1	B	50	ASP	C-O	-5.02	1.18	1.24
1	A	103	CYS	C-O	-5.01	1.17	1.24
1	A	204	GLY	C-O	-5.01	1.17	1.23
1	B	115	ASP	C-O	-5.00	1.17	1.23
1	B	288	VAL	C-O	-5.00	1.18	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	PRO	CA-C-N	-10.76	109.76	120.31
1	B	295	PRO	C-N-CA	-10.76	109.76	120.31
1	A	324	SER	N-CA-C	8.22	119.86	111.07
1	B	324	SER	N-CA-C	8.16	119.80	111.07
1	B	323	LYS	N-CA-C	-6.32	100.31	109.59
1	B	284	GLU	N-CA-C	6.20	119.94	112.38
1	B	299[A]	GLN	CA-C-O	6.09	127.38	120.80
1	B	299[B]	GLN	CA-C-O	6.09	127.38	120.80
1	A	298	SER	N-CA-C	5.89	120.05	112.86
1	A	175	GLY	N-CA-C	5.77	119.62	112.64
1	B	32	LYS	CG-CD-CE	5.77	124.56	111.30
1	A	327	SER	N-CA-C	5.75	120.44	112.45
1	A	323	LYS	N-CA-C	-5.66	101.27	109.59
1	B	327	SER	N-CA-C	5.63	120.27	112.45
1	B	295	PRO	CB-CA-C	-5.58	104.11	110.92
1	B	164	SER	N-CA-C	5.54	116.68	109.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	SER	N-CA-C	5.37	122.23	110.80
1	B	69	ALA	N-CA-C	5.21	116.21	108.60
1	A	246	TYR	N-CA-C	5.17	118.00	109.72
1	B	326	ASP	CB-CA-C	-5.14	102.11	110.85
1	A	284	GLU	N-CA-C	5.13	117.61	111.71
1	B	291	ILE	CB-CA-C	-5.11	104.57	110.91
1	B	296	PRO	CA-C-O	5.11	128.46	122.12
1	B	246	TYR	N-CA-C	5.06	117.99	109.95
1	A	17	GLU	N-CA-C	5.03	117.19	110.35
1	B	294	VAL	CB-CA-C	-5.02	105.00	110.78

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	2788	0	2849	38	0
1	B	2797	0	2862	43	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	25	1	0
3	B	44	0	25	1	0
4	A	9	0	13	2	0
4	B	9	0	13	2	0
5	A	308	0	0	3	0
5	B	245	0	0	5	0
All	All	6248	0	5787	74	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 6.

All (74) 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:81:THR:HA	1:A:84:ARG:HH12	1.46	0.81
1:A:101:ARG:HH21	1:B:283:GLN:HE21	1.29	0.81
1:A:10:LYS:HE3	1:A:148:GLN:CD	2.09	0.77
1:B:16:GLU:HG3	1:B:19:LYS:HG3	1.67	0.76
1:A:10:LYS:HG2	1:A:148:GLN:CG	2.18	0.73
1:B:248:LYS:HB2	1:B:249:PRO:CD	2.19	0.73
1:A:318:ILE:HD13	1:B:309:LEU:HD13	1.71	0.72
1:A:226:LYS:HZ3	1:A:242:ASN:HB2	1.55	0.70
1:A:185:LYS:NZ	5:A:502:HOH:O	2.25	0.69
1:A:271:ARG:O	1:A:275:MET:HG3	1.94	0.67
1:A:10:LYS:HG2	1:A:148:GLN:CD	2.20	0.66
1:B:32:LYS:HD2	1:B:129:ARG:NH2	2.14	0.62
1:A:10:LYS:HG2	1:A:148:GLN:HG3	1.81	0.62
1:B:226:LYS:NZ	1:B:245:ASP:OD2	2.30	0.61
1:A:318:ILE:CD1	1:B:309:LEU:HD13	2.31	0.61
1:B:131:THR:HG23	5:B:649:HOH:O	2.00	0.60
1:A:226:LYS:HZ3	1:A:242:ASN:CB	2.14	0.60
1:A:318:ILE:HD13	1:B:309:LEU:CD1	2.31	0.60
1:B:228:LYS:HE2	1:B:368:ILE:HD13	1.84	0.58
1:A:101:ARG:NH2	1:B:283:GLN:HE21	2.00	0.58
1:A:83:VAL:C	1:A:84:ARG:HD3	2.28	0.57
1:B:248:LYS:HB2	1:B:249:PRO:HD2	1.86	0.57
1:A:349:VAL:C	1:A:350:LEU:HD12	2.31	0.56
1:A:318:ILE:CD1	1:B:309:LEU:CD1	2.84	0.56
1:B:365:GLY:HA2	5:B:574:HOH:O	2.05	0.55
1:B:294:VAL:HG21	4:B:404:CXF:H52	1.89	0.55
1:B:226:LYS:HE2	1:B:242:ASN:CB	2.38	0.54
1:A:365:GLY:HA2	5:A:544:HOH:O	2.07	0.54
1:B:359:PHE:O	1:B:363:ARG:HG3	2.07	0.54
1:B:301:LEU:C	1:B:301:LEU:HD12	2.35	0.52
1:B:275:MET:HE1	1:B:295:PRO:HD3	1.92	0.51
5:A:643:HOH:O	1:B:105:HIS:HE1	1.92	0.51
1:B:226:LYS:CE	1:B:242:ASN:HD22	2.25	0.49
1:B:226:LYS:CE	1:B:245:ASP:OD2	2.61	0.48
1:A:350:LEU:HD13	1:A:370:THR:HG23	1.95	0.48
1:B:294:VAL:HG23	3:B:403:NAI:H1D	1.96	0.48
1:A:67:HIS:CD2	4:A:404:CXF:H7	2.50	0.47
1:A:17:GLU:H	1:A:17:GLU:CD	2.23	0.46
1:A:56:THR:HG23	1:A:296:PRO:HA	1.97	0.46
1:A:306:MET:HE1	1:B:294:VAL:HG13	1.98	0.46
1:B:40:MET:HA	1:B:40:MET:HE2	1.96	0.46
1:A:10:LYS:HG2	1:A:148:GLN:OE1	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PRO:CD	1:B:306:MET:HE3	2.46	0.46
1:B:27:GLU:OE1	1:B:131:THR:OG1	2.34	0.46
1:A:10:LYS:HE3	1:A:148:GLN:NE2	2.31	0.45
1:B:226:LYS:HE2	1:B:242:ASN:HB3	1.97	0.45
1:A:40:MET:HA	1:A:40:MET:HE2	1.99	0.45
1:A:226:LYS:NZ	1:A:242:ASN:HB2	2.30	0.45
1:A:364:SER:OG	1:A:366:GLU:HG2	2.17	0.45
1:B:105:HIS:HD2	1:B:107:GLU:H	1.63	0.45
1:B:32:LYS:HD2	1:B:129:ARG:CZ	2.46	0.44
1:B:105:HIS:CD2	1:B:107:GLU:H	2.35	0.44
1:A:209:MET:HE2	1:A:209:MET:HB3	1.85	0.44
1:A:10:LYS:CG	1:A:148:GLN:CG	2.94	0.44
1:A:226:LYS:NZ	1:A:242:ASN:CB	2.81	0.44
1:B:167:GLU:H	1:B:167:GLU:CD	2.26	0.44
1:A:191:GLN:HG2	1:A:215:GLY:HA3	1.99	0.43
1:B:228:LYS:HD3	1:B:368:ILE:HD11	1.99	0.43
1:B:116:LEU:HD21	4:B:404:CXF:H41	2.00	0.43
1:A:294:VAL:HG21	4:A:404:CXF:H52	2.01	0.43
1:B:271:ARG:O	1:B:275:MET:HG3	2.18	0.43
1:A:10:LYS:CG	1:A:148:GLN:HG3	2.48	0.43
1:B:357:GLU:HG2	5:B:734:HOH:O	2.17	0.43
1:B:363:ARG:HD2	5:B:613:HOH:O	2.19	0.43
1:B:38:ILE:CG2	1:B:40:MET:CE	2.97	0.42
3:A:403:NAI:H6N	3:A:403:NAI:H2D	1.83	0.42
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.20	0.42
1:A:15:TRP:HA	1:A:62:PRO:HB3	2.02	0.42
1:B:228:LYS:HB3	5:B:547:HOH:O	2.20	0.41
1:B:123:MET:HE3	1:B:123:MET:HB3	1.98	0.41
1:B:10:LYS:HD2	1:B:10:LYS:HA	1.89	0.41
1:B:343:ASP:N	1:B:344:PRO:CD	2.84	0.41
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.21	0.41
1:A:84:ARG:HD3	1:A:84:ARG:N	2.37	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	372/377 (99%)	356 (96%)	15 (4%)	1 (0%)	36	21
1	B	374/377 (99%)	361 (96%)	13 (4%)	0	100	100
All	All	746/754 (99%)	717 (96%)	28 (4%)	1 (0%)	48	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	ILE

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	308/308 (100%)	308 (100%)	0	100	100
1	B	310/308 (101%)	307 (99%)	3 (1%)	68	52
All	All	618/616 (100%)	615 (100%)	3 (0%)	86	72

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	268	VAL
1	B	299[A]	GLN
1	B	299[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	300	ASN
1	B	105	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	191	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 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	$\# Z > 2$
4	CXF	B	404	2	9,9,9	1.26	2 (22%)	9,10,10	2.18	5 (55%)
3	NAI	A	403	-	47,48,48	3.59	25 (53%)	64,73,73	1.86	10 (15%)
4	CXF	A	404	2	9,9,9	1.76	2 (22%)	9,10,10	1.81	2 (22%)
3	NAI	B	403	-	47,48,48	3.68	28 (59%)	64,73,73	1.73	11 (17%)

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	CXF	B	404	2	-	0/3/11/11	0/1/1/1
3	NAI	A	403	-	-	5/29/72/72	0/5/5/5
4	CXF	A	404	2	-	0/3/11/11	0/1/1/1
3	NAI	B	403	-	-	4/29/72/72	0/5/5/5

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	NAI	O4D-C1D	7.87	1.60	1.42
3	B	403	NAI	O4B-C1B	7.64	1.59	1.42
3	A	403	NAI	O4B-C1B	7.63	1.59	1.42
3	B	403	NAI	O4D-C1D	7.39	1.59	1.42
3	A	403	NAI	C2B-C1B	-7.20	1.30	1.53
3	B	403	NAI	C2B-C1B	-7.16	1.31	1.53
3	B	403	NAI	O4B-C4B	-7.10	1.29	1.45
3	A	403	NAI	O4B-C4B	-7.09	1.29	1.45
3	A	403	NAI	C2D-C1D	-6.85	1.32	1.53
3	A	403	NAI	O4D-C4D	-6.79	1.29	1.45
3	B	403	NAI	O4D-C4D	-6.79	1.29	1.45
3	B	403	NAI	C2D-C1D	-6.71	1.32	1.53
3	A	403	NAI	C2N-C3N	6.44	1.52	1.35
3	B	403	NAI	C2N-C3N	5.91	1.51	1.35
3	B	403	NAI	PA-O3	5.86	1.65	1.59
3	B	403	NAI	O7N-C7N	-5.12	1.12	1.24
3	A	403	NAI	C7N-N7N	4.98	1.47	1.33
3	A	403	NAI	O7N-C7N	-4.92	1.12	1.24
3	A	403	NAI	C5A-C4A	-4.79	1.30	1.39
3	B	403	NAI	C6N-C5N	4.67	1.47	1.33
3	A	403	NAI	C6N-C5N	4.64	1.47	1.33
4	A	404	CXF	C1-N8	-4.58	1.42	1.47
3	A	403	NAI	O3D-C3D	-4.56	1.31	1.43
3	B	403	NAI	C5A-N7A	-4.26	1.31	1.39
3	A	403	NAI	PN-O2N	-4.06	1.36	1.50
3	B	403	NAI	C7N-N7N	4.00	1.45	1.33
3	B	403	NAI	C8A-N9A	-3.95	1.30	1.37
3	B	403	NAI	O2B-C2B	3.82	1.52	1.43
3	A	403	NAI	C5A-N7A	-3.79	1.32	1.39
3	B	403	NAI	C5A-C4A	-3.65	1.32	1.39
3	B	403	NAI	C6A-N6A	3.59	1.43	1.34
3	B	403	NAI	O3D-C3D	-3.55	1.34	1.43
3	A	403	NAI	C8A-N9A	-3.36	1.31	1.37
3	B	403	NAI	O3B-C3B	-3.34	1.34	1.43
3	B	403	NAI	PA-O2A	-3.16	1.40	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	NAI	PN-O2N	-3.14	1.39	1.50
3	A	403	NAI	O3B-C3B	-3.06	1.35	1.43
3	A	403	NAI	C6A-N6A	2.91	1.41	1.34
3	B	403	NAI	C4A-N9A	-2.88	1.31	1.37
3	A	403	NAI	PA-O2A	-2.86	1.42	1.55
3	B	403	NAI	C6A-N1A	-2.80	1.27	1.35
3	A	403	NAI	O5D-C5D	-2.75	1.34	1.44
3	B	403	NAI	C7N-C3N	2.69	1.54	1.48
3	B	403	NAI	PA-O1A	-2.57	1.41	1.50
3	A	403	NAI	O5B-C5B	-2.47	1.35	1.44
3	A	403	NAI	C6A-N1A	-2.42	1.29	1.35
3	A	403	NAI	C4A-N9A	-2.36	1.32	1.37
3	B	403	NAI	C3B-C4B	2.31	1.58	1.53
3	A	403	NAI	O2B-C2B	2.23	1.48	1.43
4	B	404	CXF	C1-N8	-2.20	1.45	1.47
3	A	403	NAI	C6N-N1N	2.10	1.42	1.37
3	A	403	NAI	PN-O1N	-2.09	1.45	1.55
3	B	403	NAI	O5D-C5D	-2.08	1.36	1.44
4	B	404	CXF	O9-C7	-2.08	1.14	1.22
3	B	403	NAI	PN-O5D	2.07	1.67	1.59
3	B	403	NAI	O5B-C5B	-2.02	1.37	1.44
4	A	404	CXF	O9-C7	-2.02	1.14	1.22

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	NAI	N3A-C2A-N1A	-5.85	119.72	128.58
3	A	403	NAI	C5A-C4A-N3A	-5.61	118.99	126.72
3	B	403	NAI	N3A-C2A-N1A	-5.22	120.68	128.58
3	B	403	NAI	C5A-C4A-N3A	-5.08	119.72	126.72
3	A	403	NAI	N6A-C6A-N1A	-5.01	107.22	118.38
3	B	403	NAI	N6A-C6A-N1A	-4.95	107.35	118.38
3	B	403	NAI	N3A-C4A-N9A	3.94	133.86	127.17
3	A	403	NAI	N9A-C8A-N7A	-3.82	108.51	113.94
3	A	403	NAI	N3A-C4A-N9A	3.73	133.51	127.17
3	A	403	NAI	C5A-C6A-N6A	3.73	132.52	123.29
4	A	404	CXF	C6-C1-C2	-3.53	104.71	110.80
3	B	403	NAI	C2A-N3A-C4A	3.43	120.21	111.83
3	B	403	NAI	C5A-C6A-N6A	3.38	131.66	123.29
3	A	403	NAI	C2A-N3A-C4A	3.35	120.01	111.83
4	B	404	CXF	C6-C1-C2	-3.32	105.07	110.80
3	A	403	NAI	O4B-C1B-C2B	-3.22	99.72	106.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	CXF	C3-C2-C1	3.08	116.61	111.09
3	B	403	NAI	O3-PA-O1A	-2.84	102.17	110.70
3	B	403	NAI	C3N-C2N-N1N	-2.80	119.10	123.20
4	B	404	CXF	C5-C6-C1	-2.57	106.49	111.09
3	A	403	NAI	C5A-N7A-C8A	2.43	107.27	103.45
4	B	404	CXF	O9-C7-N8	-2.34	119.28	125.32
4	A	404	CXF	O9-C7-N8	-2.17	119.71	125.32
4	B	404	CXF	C5-C4-C3	-2.14	104.83	111.19
3	B	403	NAI	C5B-C4B-C3B	-2.09	107.70	115.21
3	B	403	NAI	O2A-PA-O1A	2.08	122.10	112.44
3	A	403	NAI	O2A-PA-O3	2.04	112.79	107.27
3	B	403	NAI	C2D-C1D-N1N	2.04	118.33	113.31

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

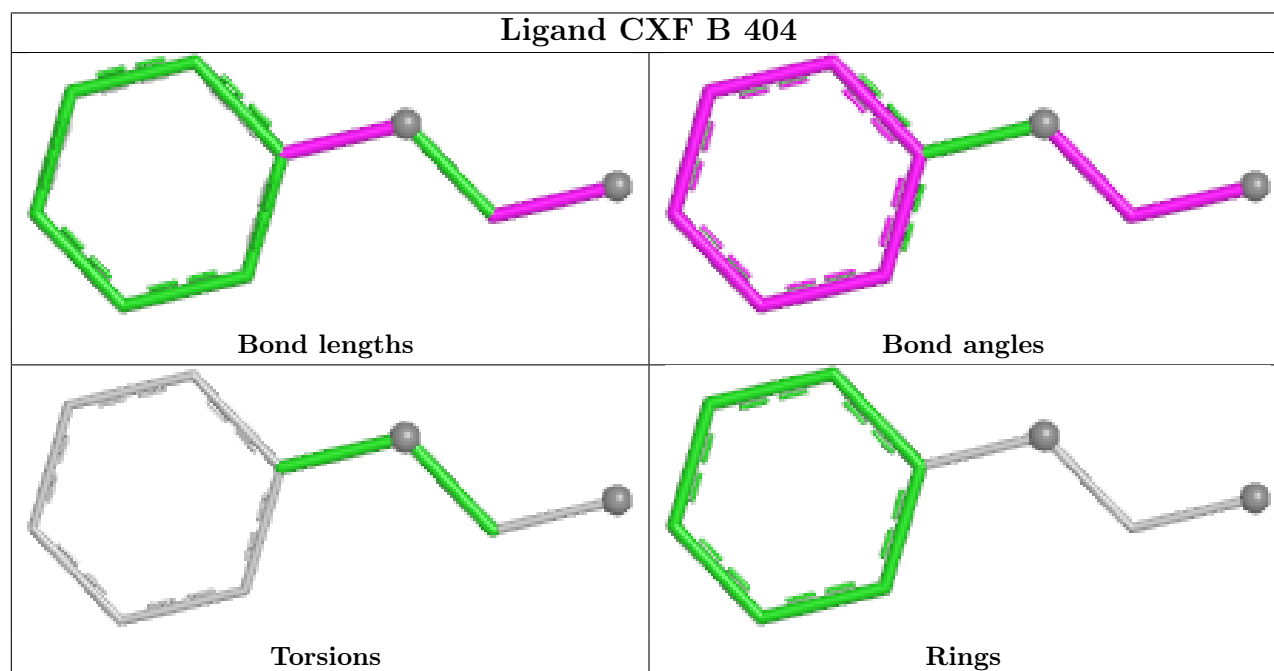
There are no ring outliers.

4 monomers are involved in 6 short contacts:

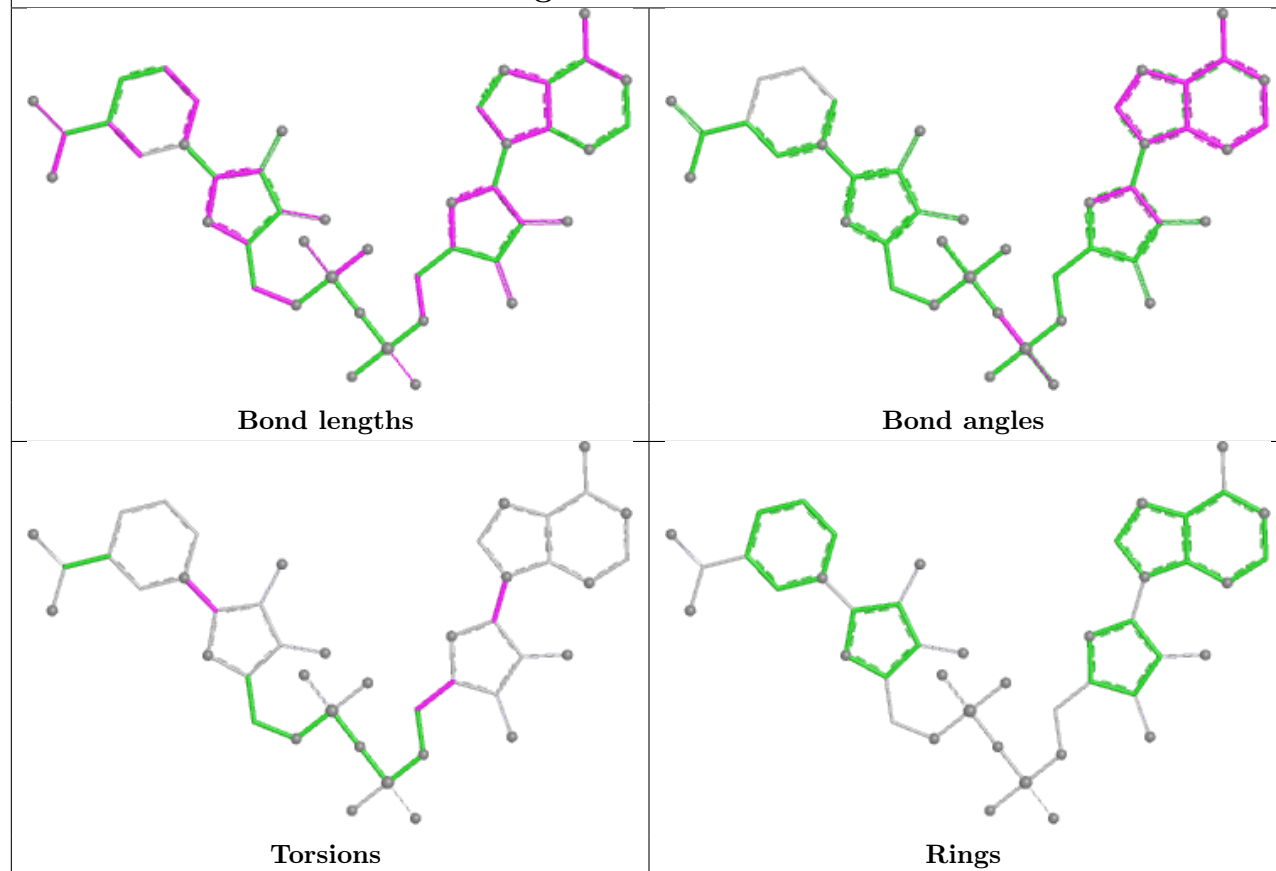
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	404	CXF	2	0
3	A	403	NAI	1	0
4	A	404	CXF	2	0
3	B	403	NAI	1	0

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

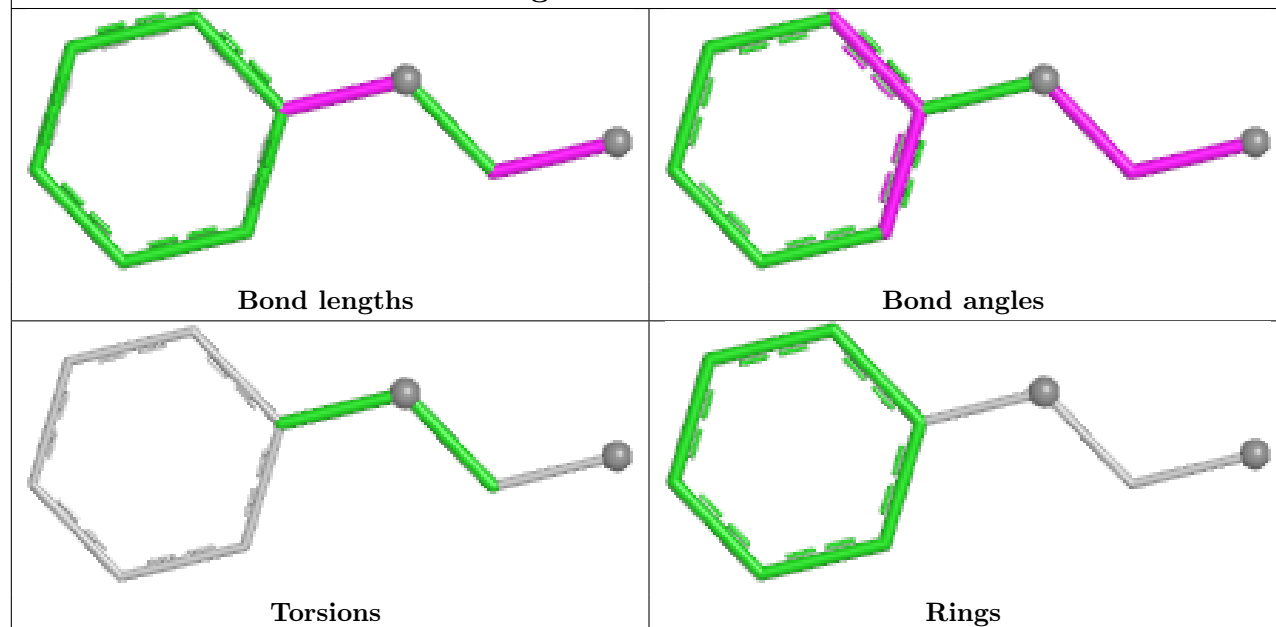
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

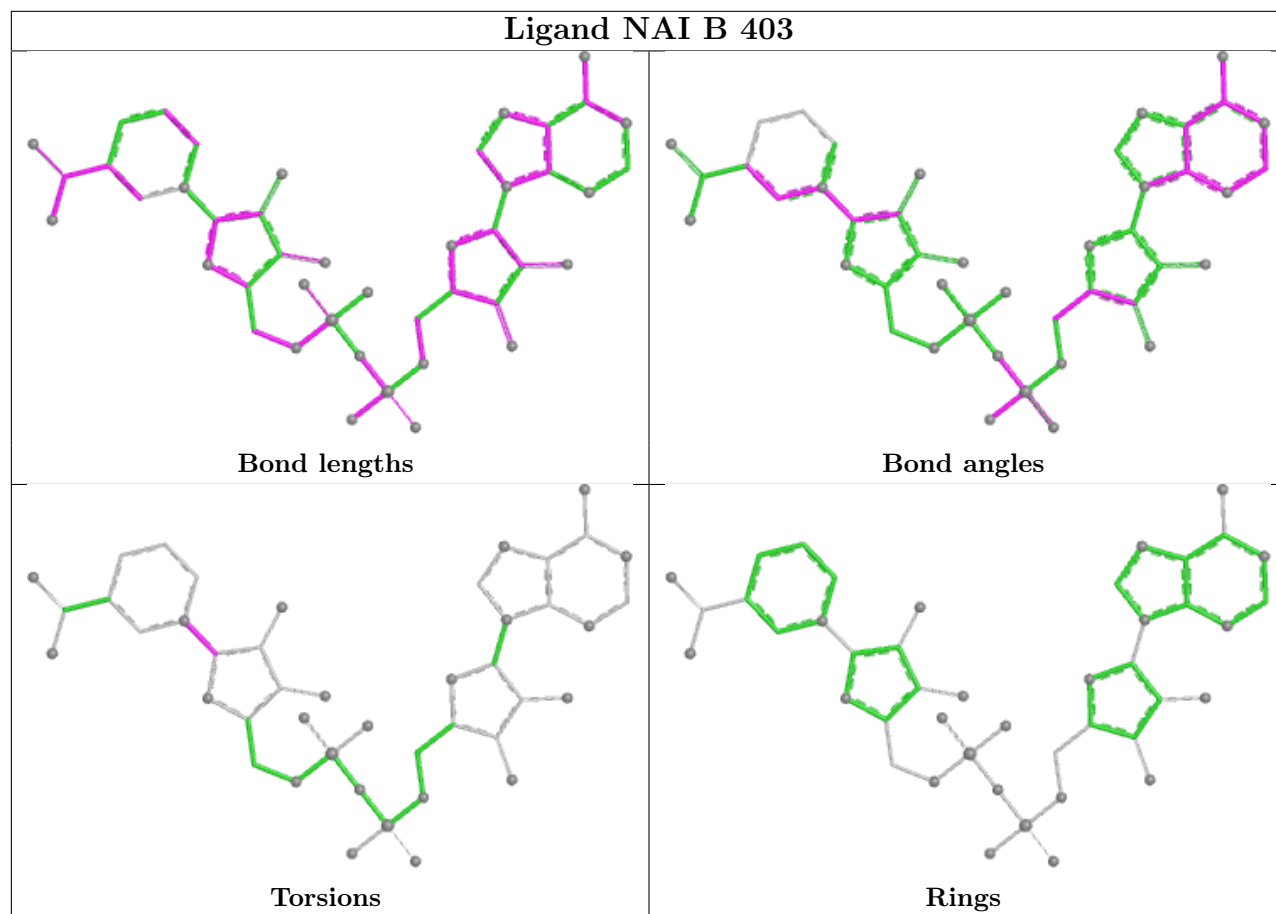


Ligand NAI A 403



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%)	0.09	5 (1%) 75 80	9, 14, 24, 35	0
1	B	374/377 (99%)	0.18	4 (1%) 78 83	9, 15, 27, 64	2 (0%)
All	All	748/754 (99%)	0.14	9 (1%) 76 81	9, 14, 26, 64	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	PRO	4.4
1	B	298	SER	3.9
1	B	297	ASP	3.8
1	B	299[A]	GLN	2.6
1	A	298	SER	2.5
1	A	84	ARG	2.4
1	A	1	SER	2.4
1	A	366	GLU	2.1
1	A	101	ARG	2.1

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.

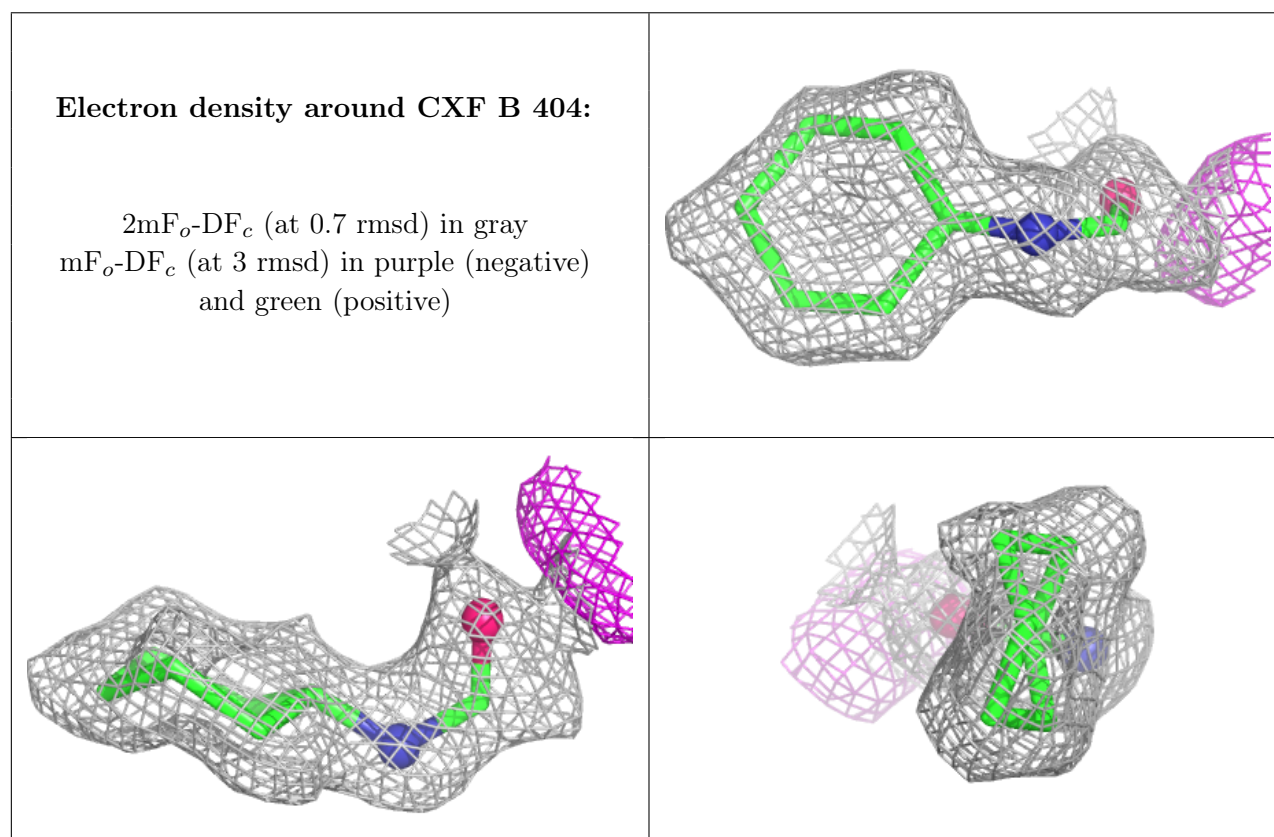
6.4 Ligands [i](#)

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.

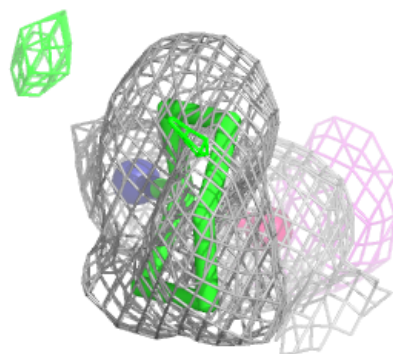
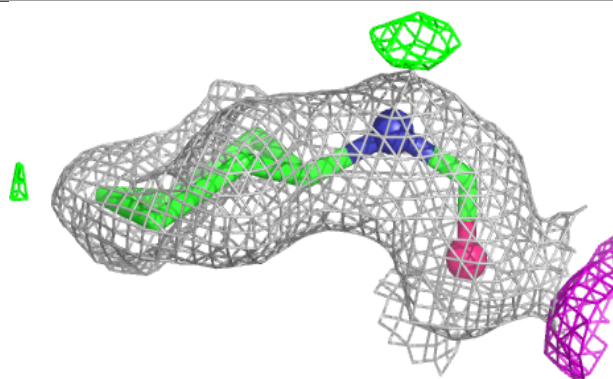
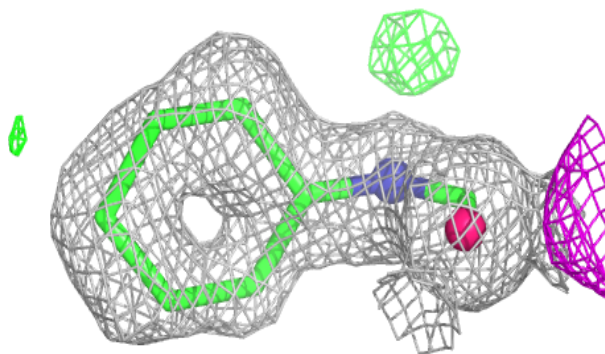
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CXF	B	404	9/9	0.91	0.08	19,19,20,21	0
4	CXF	A	404	9/9	0.94	0.08	18,19,20,20	0
3	NAI	A	403	44/44	0.96	0.06	9,12,14,14	0
3	NAI	B	403	44/44	0.96	0.07	11,13,14,14	0
2	ZN	B	401	1/1	0.98	0.12	21,21,21,21	0
2	ZN	A	401	1/1	0.99	0.10	21,21,21,21	0
2	ZN	B	402	1/1	0.99	0.03	12,12,12,12	0
2	ZN	A	402	1/1	0.99	0.02	12,12,12,12	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.

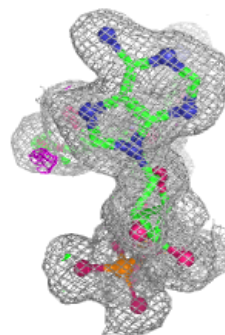
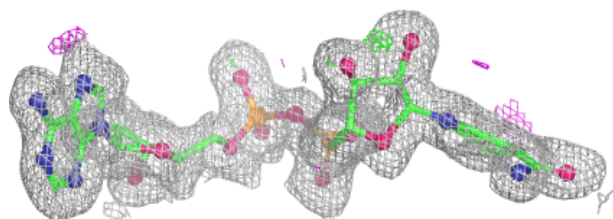
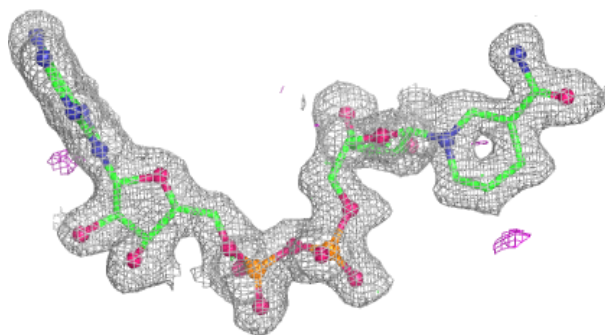


Electron density around CXF A 404:

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

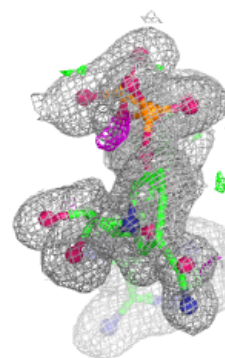
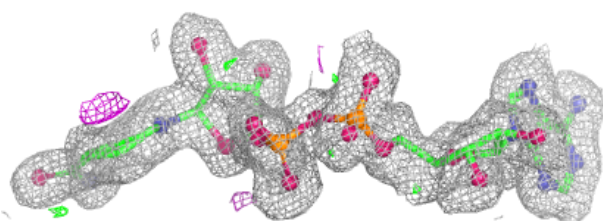
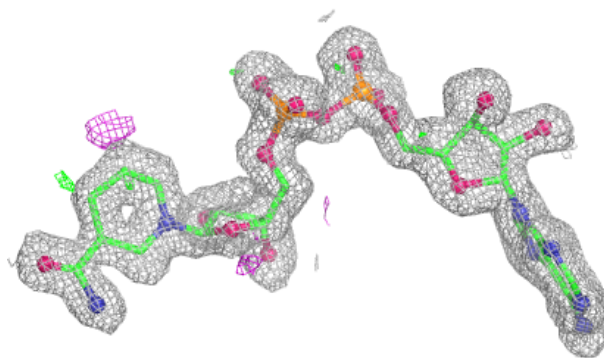
**Electron density around NAI A 403:**

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



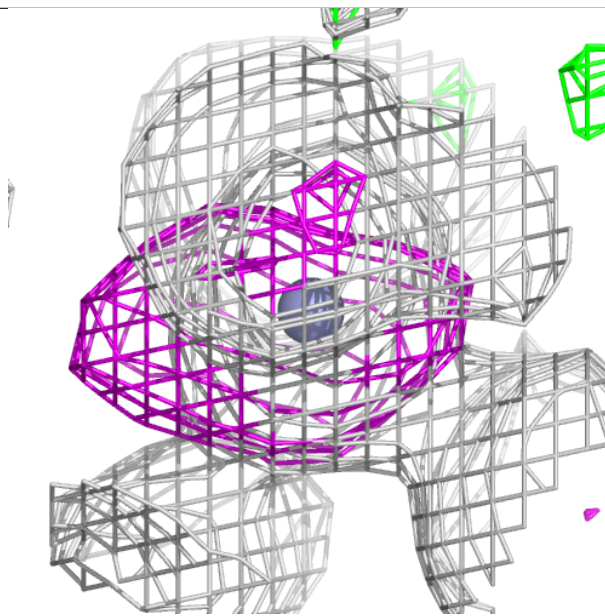
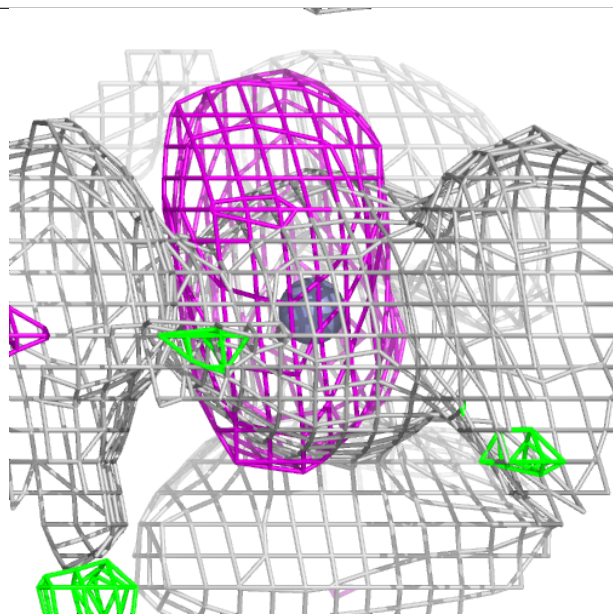
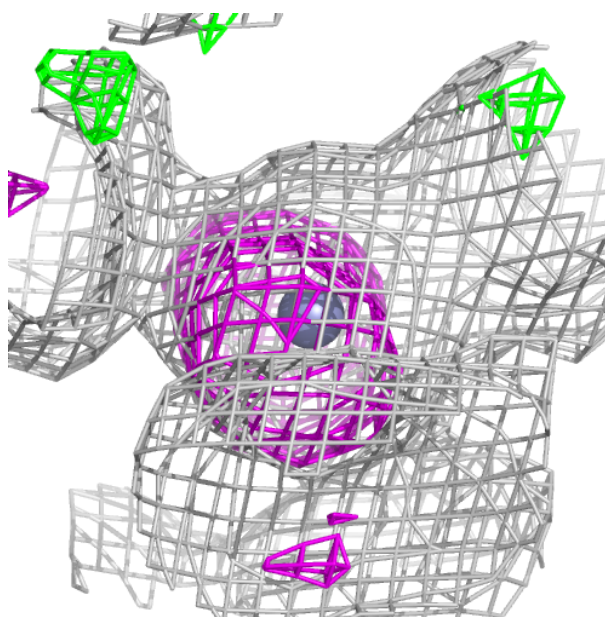
Electron density around NAI B 403:

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



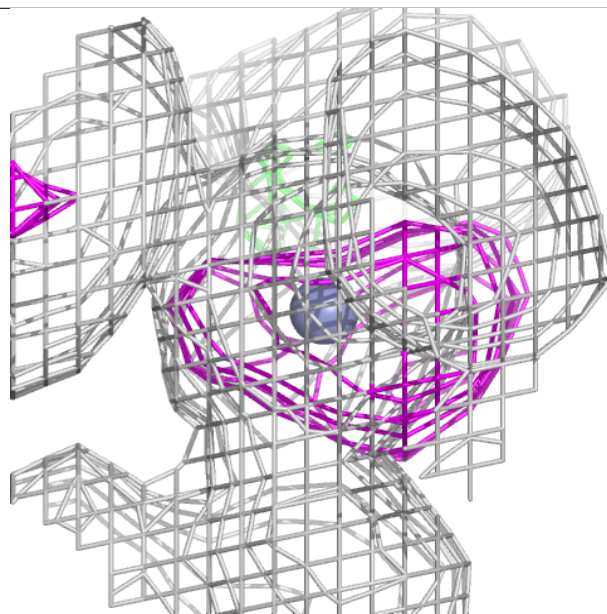
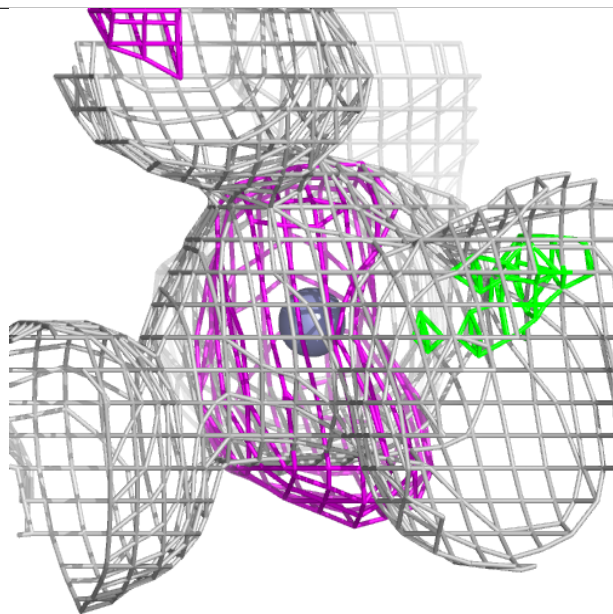
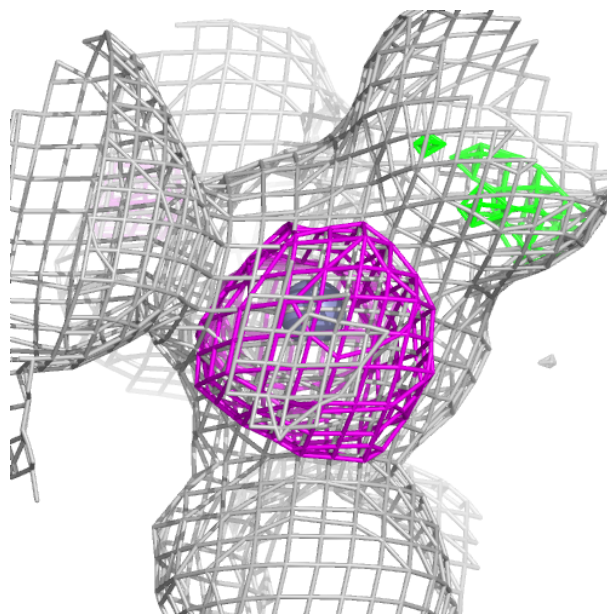
Electron density around ZN B 401:

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



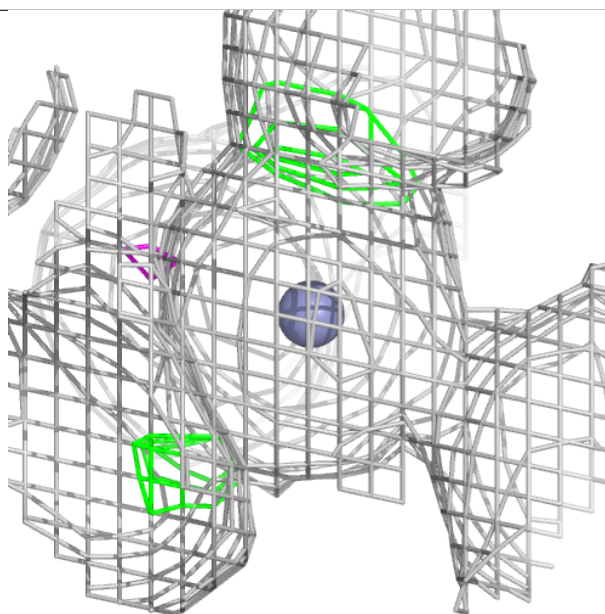
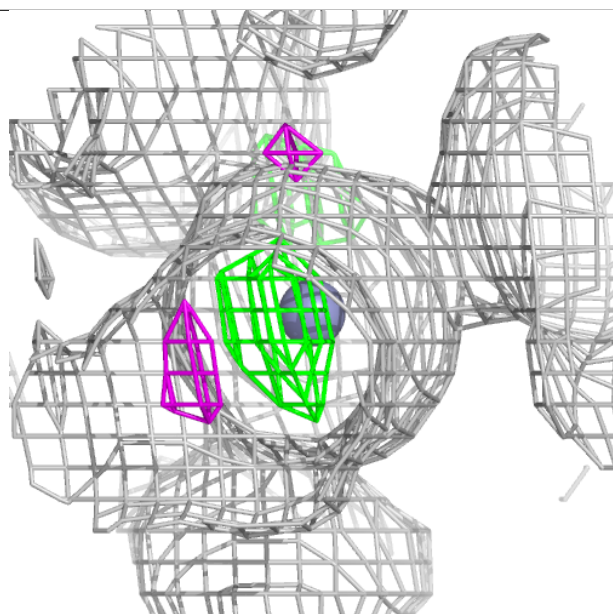
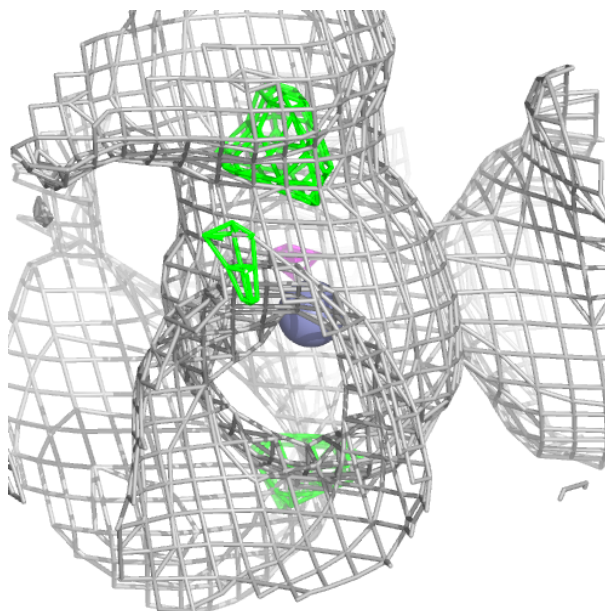
Electron density around ZN A 401:

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



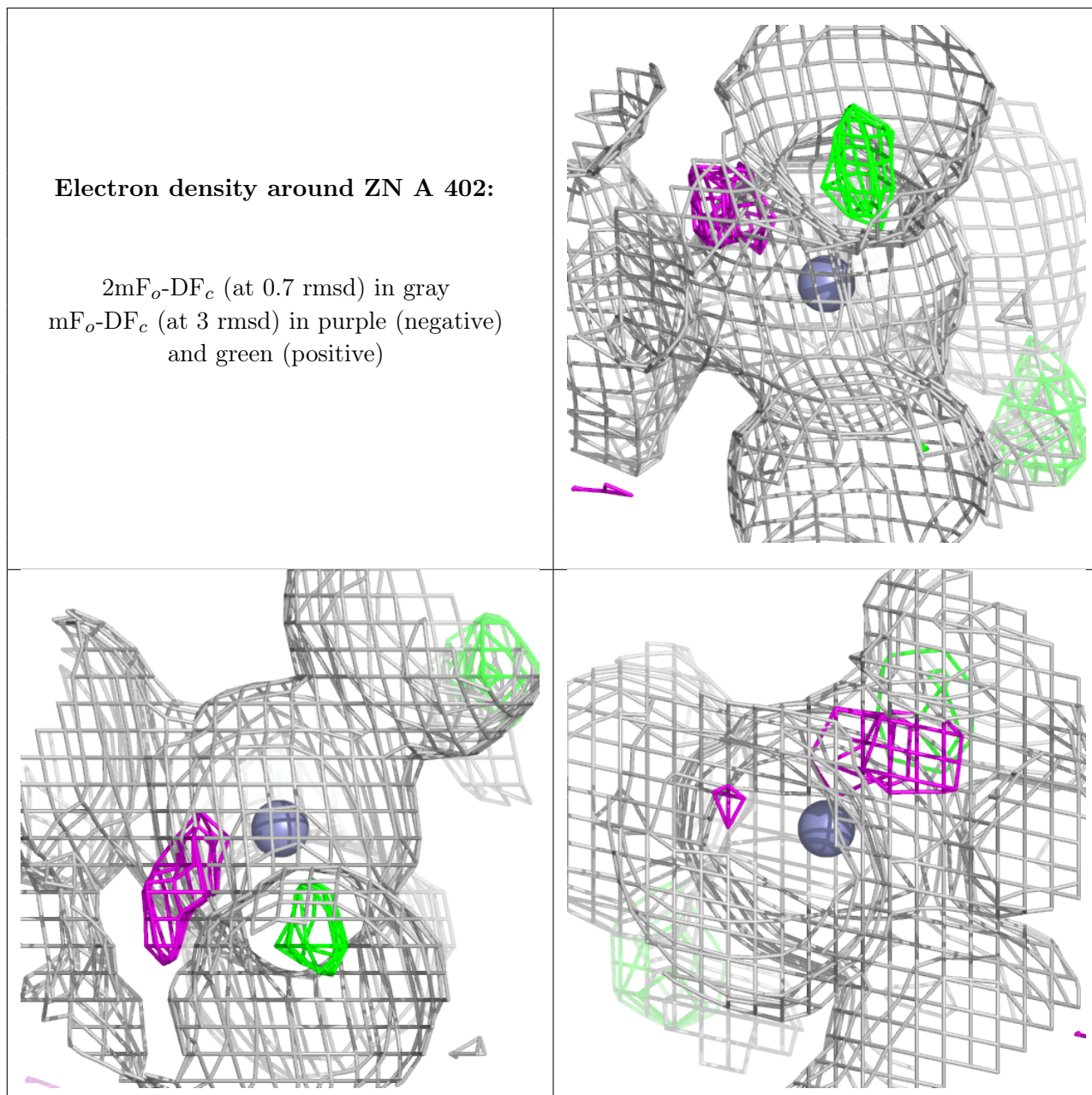
Electron density around ZN B 402:

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



Electron density around ZN A 402:

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

**6.5 Other polymers** ⓘ

There are no such residues in this entry.