



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:58 PM UTC

PDB ID : 8FW6 / pdb_00008fw6
Title : Human Lactate Dehydrogenase A in Complex with Inhibitor CHK-336
Authors : Lowther, W.T.; Gumpena, R.
Deposited on : 2023-01-20
Resolution : 2.34 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

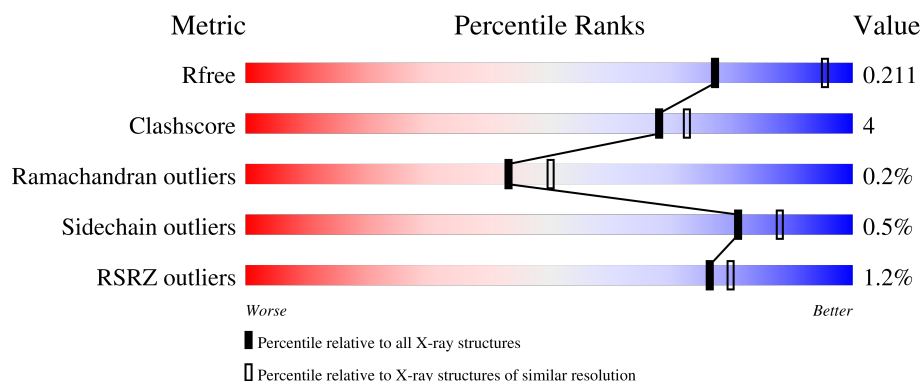
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	338	% 92% 5% ..
1	B	338	% 88% 9% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5694 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.

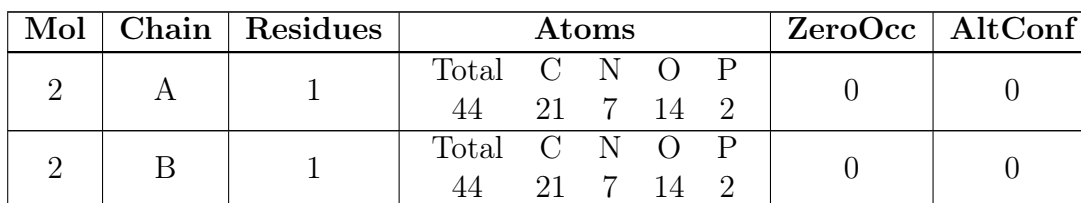
- Molecule 1 is a protein called L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	1	0
			2568	1639	439	477	13			
1	B	331	Total	C	N	O	S	0	1	0
			2567	1638	438	478	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	HIS	-	expression tag	UNP P00338
A	334	HIS	-	expression tag	UNP P00338
A	335	HIS	-	expression tag	UNP P00338
A	336	HIS	-	expression tag	UNP P00338
A	337	HIS	-	expression tag	UNP P00338
A	338	HIS	-	expression tag	UNP P00338
B	333	HIS	-	expression tag	UNP P00338
B	334	HIS	-	expression tag	UNP P00338
B	335	HIS	-	expression tag	UNP P00338
B	336	HIS	-	expression tag	UNP P00338
B	337	HIS	-	expression tag	UNP P00338
B	338	HIS	-	expression tag	UNP P00338

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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- The ORTEP diagram illustrates the molecular structure of YBO. The molecule features a central benzimidazole core. A 2-(cyclopropylmethyl)-5-(4-fluorophenyl)benzimidazole moiety is attached to the 2-position of the benzimidazole ring. The cyclopropyl group is represented by atoms C12, C13, and C14, with C15 indicating a displacement. The 4-fluorophenyl group consists of a benzene ring with atoms C05 through C09 and a fluorine atom F36. The benzimidazole ring system includes atoms N01, N16, N18, N25, and N26. A 2-(4-fluorophenyl)-5-(4-fluorophenyl)benzimidazole moiety is attached to the 5-position of the benzimidazole ring. This moiety includes a benzene ring with atoms C20 through C24 and a fluorine atom F31. The displacement ellipsoids are drawn at the 50% probability level, and the structure is shown with thermal ellipsoids at the 50% probability level.

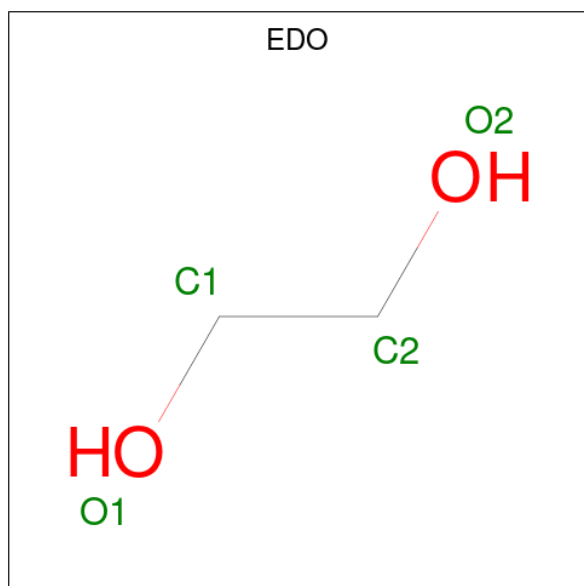
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			36	24	2	4	4	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	S	
			36	24	2	4	4	2	
								0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



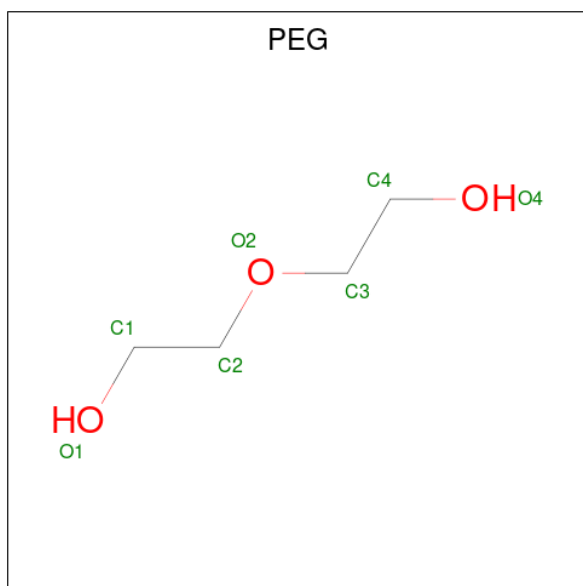
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O		
			4	2	2	0	0
4	A	1	Total	C	O		
			4	2	2	0	0
4	A	1	Total	C	O		
			4	2	2	0	0
4	A	1	Total	C	O		
			4	2	2	0	0
4	A	1	Total	C	O		
			4	2	2	0	0
4	A	1	Total	C	O		
			4	2	2	0	0
4	A	1	Total	C	O		
			4	2	2	0	0
4	A	1	Total	C	O		
			4	2	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	183	Total	O	0	0
			183	183		

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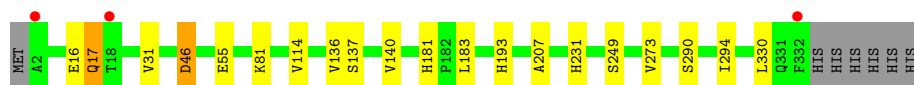
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	141	Total 141	O 141	0	0

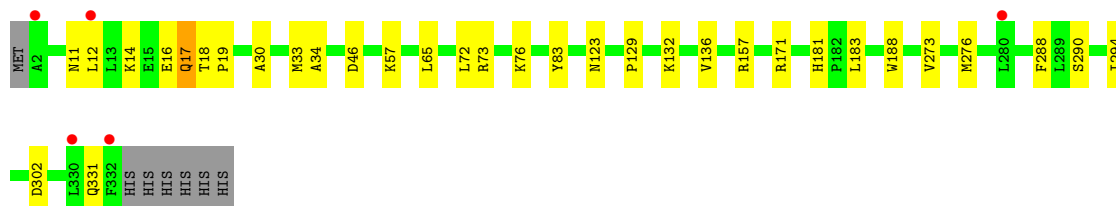
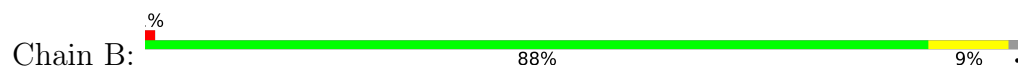
3 Residue-property plots [i](#)

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: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.17Å 118.17Å 94.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.07 – 2.34 45.07 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.07-2.34) 99.4 (45.07-2.34)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, R_{free}	0.154 , 0.206 0.164 , 0.211	Depositor DCC
R_{free} test set	1562 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5694	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: PEG, NAI, EDO, YBO

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	0.66	2/2615 (0.1%)	0.99	1/3539 (0.0%)
1	B	0.60	0/2611	0.99	1/3534 (0.0%)
All	All	0.63	2/5226 (0.0%)	0.99	2/7073 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	HIS	CE1-NE2	6.09	1.38	1.32
1	A	193	HIS	CE1-NE2	5.26	1.37	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ASP	CA-CB-CG	6.69	119.29	112.60
1	B	46	ASP	CA-CB-CG	6.38	118.98	112.60

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	2568	0	2648	12	0
1	B	2567	0	2639	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	26	4	0
2	B	44	0	26	2	0
3	A	36	0	0	2	0
3	B	36	0	0	1	0
4	A	44	0	66	1	0
4	B	24	0	36	8	0
5	B	7	0	10	0	0
6	A	183	0	0	1	0
6	B	141	0	0	3	0
All	All	5694	0	5451	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 4.

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:A:46:ASP:HB3	6:A:618:HOH:O	1.82	0.79
1:B:294:ILE:HD12	1:B:302:ASP:HB2	1.81	0.63
1:B:171:ARG:HH11	4:B:406:EDO:H22	1.63	0.62
1:A:31:VAL:HG21	2:A:401:NAI:H6N	1.82	0.60
1:B:34:ALA:HB2	4:B:404:EDO:H22	1.84	0.59
2:A:401:NAI:H5N	3:A:402:YBO:C23	2.34	0.58
1:B:11:ASN:OD1	1:B:14:LYS:HD2	2.04	0.57
1:A:273:VAL:O	1:A:290:SER:HA	2.06	0.56
1:A:16:GLU:O	1:A:17:GLN:HB3	2.06	0.55
1:B:273:VAL:O	1:B:290:SER:HA	2.10	0.52
1:B:73:ARG:HG2	4:B:405:EDO:O1	2.09	0.52
1:B:132:LYS:NZ	6:B:503:HOH:O	2.39	0.52
1:A:294:ILE:N	1:A:294:ILE:HD12	2.25	0.52
1:B:136:VAL:O	2:B:401:NAI:H2N	2.10	0.50
1:B:129:PRO:O	1:B:157:ARG:NH1	2.45	0.50
1:B:18:THR:HG22	1:B:19:PRO:HD2	1.93	0.49
1:A:136:VAL:O	2:A:401:NAI:H2N	2.15	0.47
1:B:16:GLU:O	1:B:17:GLN:CB	2.63	0.45
1:B:171:ARG:NH1	4:B:406:EDO:H22	2.30	0.45
1:A:55:GLU:OE1	1:A:81:LYS:HD2	2.17	0.45
2:B:401:NAI:H42N	3:B:402:YBO:C20	2.47	0.44
2:A:401:NAI:C5N	3:A:402:YBO:C23	2.96	0.44
1:A:114:VAL:HG21	1:A:330:LEU:HD13	2.00	0.43
1:B:57:LYS:NZ	6:B:510:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:SER:HB2	4:A:407:EDO:H22	2.00	0.43
1:B:181:HIS:CE1	1:B:183:LEU:HD12	2.55	0.42
1:B:76:LYS:HA	4:B:409:EDO:H12	2.01	0.42
1:B:171:ARG:HH11	4:B:406:EDO:C2	2.29	0.41
1:B:294:ILE:HD12	1:B:302:ASP:CB	2.50	0.41
1:B:33:MET:HE1	1:B:65:LEU:HD11	2.03	0.41
1:B:30:ALA:O	4:B:404:EDO:C2	2.68	0.41
1:A:207:ALA:HA	1:B:188:TRP:CE2	2.56	0.41
1:B:30:ALA:O	4:B:404:EDO:H21	2.20	0.41
1:A:137:SER:O	1:A:140:VAL:HA	2.22	0.40
1:B:83:TYR:CG	1:B:123:ASN:HB3	2.56	0.40
1:A:181:HIS:CE1	1:A:183:LEU:HD12	2.56	0.40
1:B:72:LEU:O	1:B:73:ARG:HD3	2.21	0.40
1:B:157:ARG:HD3	6:B:587:HOH:O	2.20	0.40
1:B:276:MET:HG2	1:B:288:PHE:CE1	2.57	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	330/338 (98%)	322 (98%)	8 (2%)	0	100	100
1	B	330/338 (98%)	321 (97%)	8 (2%)	1 (0%)	36	41
All	All	660/676 (98%)	643 (97%)	16 (2%)	1 (0%)	43	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	GLN

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	287/294 (98%)	286 (100%)	1 (0%)	86	91
1	B	286/294 (97%)	284 (99%)	2 (1%)	76	84
All	All	573/588 (97%)	570 (100%)	3 (0%)	81	88

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

Mol	Chain	Res	Type
1	A	17	GLN
1	B	12	LEU
1	B	331	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	HIS
1	A	233	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

22 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
5	PEG	B	403	-	6,6,6	0.21	0	5,5,5	0.13	0
4	EDO	B	409	-	3,3,3	0.29	0	2,2,2	0.33	0
3	YBO	B	402	-	40,40,40	2.35	14 (35%)	54,60,60	2.74	23 (42%)
4	EDO	A	412	-	3,3,3	0.12	0	2,2,2	0.16	0
4	EDO	B	408	-	3,3,3	0.12	0	2,2,2	0.42	0
2	NAI	A	401	-	47,48,48	3.19	21 (44%)	64,73,73	1.83	17 (26%)
4	EDO	A	408	-	3,3,3	0.20	0	2,2,2	0.34	0
4	EDO	B	407	-	3,3,3	0.15	0	2,2,2	0.15	0
4	EDO	B	404	-	3,3,3	0.05	0	2,2,2	0.47	0
3	YBO	A	402	-	40,40,40	2.48	11 (27%)	54,60,60	2.32	16 (29%)
2	NAI	B	401	-	47,48,48	3.29	22 (46%)	64,73,73	2.04	23 (35%)
4	EDO	B	406	-	3,3,3	0.21	0	2,2,2	0.21	0
4	EDO	A	409	-	3,3,3	0.28	0	2,2,2	0.23	0
4	EDO	A	405	-	3,3,3	0.05	0	2,2,2	0.04	0
4	EDO	A	403	-	3,3,3	0.24	0	2,2,2	0.39	0
4	EDO	A	407	-	3,3,3	0.37	0	2,2,2	0.20	0
4	EDO	A	406	-	3,3,3	0.10	0	2,2,2	0.20	0
4	EDO	A	413	-	3,3,3	0.10	0	2,2,2	0.20	0
4	EDO	A	410	-	3,3,3	0.40	0	2,2,2	0.50	0
4	EDO	A	411	-	3,3,3	0.93	0	2,2,2	0.97	0
4	EDO	B	405	-	3,3,3	0.19	0	2,2,2	0.17	0
4	EDO	A	404	-	3,3,3	0.07	0	2,2,2	0.13	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
5	PEG	B	403	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	409	-	-	0/1/1/1	-
3	YBO	B	402	-	-	1/26/28/28	0/5/5/5
4	EDO	A	412	-	-	1/1/1/1	-
4	EDO	B	408	-	-	1/1/1/1	-
2	NAI	A	401	-	-	3/29/72/72	0/5/5/5
4	EDO	A	408	-	-	1/1/1/1	-
4	EDO	B	407	-	-	1/1/1/1	-
4	EDO	B	404	-	-	1/1/1/1	-
3	YBO	A	402	-	-	1/26/28/28	0/5/5/5
2	NAI	B	401	-	-	4/29/72/72	0/5/5/5
4	EDO	B	406	-	-	1/1/1/1	-
4	EDO	A	409	-	-	0/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	A	407	-	-	1/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	A	413	-	-	0/1/1/1	-
4	EDO	A	410	-	-	1/1/1/1	-
4	EDO	A	411	-	-	1/1/1/1	-
4	EDO	B	405	-	-	1/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	YBO	C12-C11	9.84	1.54	1.49
2	A	401	NAI	C2B-C3B	-8.72	1.29	1.53
3	B	402	YBO	C12-C11	8.28	1.53	1.49
2	B	401	NAI	C2B-C3B	-8.22	1.31	1.53
2	A	401	NAI	O4D-C4D	7.31	1.61	1.45
2	B	401	NAI	O4D-C4D	7.22	1.61	1.45
2	A	401	NAI	C3D-C4D	-6.72	1.35	1.53
2	B	401	NAI	C3D-C4D	-6.31	1.37	1.53
2	B	401	NAI	PA-O3	6.30	1.66	1.59
2	B	401	NAI	C2N-C3N	6.13	1.52	1.35
2	B	401	NAI	C6N-C5N	5.75	1.50	1.33
2	B	401	NAI	O4B-C1B	-5.70	1.28	1.42
2	A	401	NAI	C2N-C3N	5.65	1.50	1.35
2	B	401	NAI	PN-O3	5.50	1.65	1.59
2	A	401	NAI	C6N-C5N	5.19	1.49	1.33
2	A	401	NAI	PA-O3	5.15	1.65	1.59
3	A	402	YBO	C27-C26	-4.98	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	YBO	S02-N01	4.83	1.69	1.60
2	B	401	NAI	O4D-C1D	-4.77	1.31	1.42
2	A	401	NAI	O4D-C1D	-4.75	1.31	1.42
3	A	402	YBO	C19-C20	4.41	1.52	1.48
2	A	401	NAI	C7N-N7N	4.37	1.46	1.33
2	A	401	NAI	O4B-C1B	-4.28	1.32	1.42
2	B	401	NAI	C2B-C1B	4.27	1.66	1.53
3	B	402	YBO	C19-C20	4.15	1.52	1.48
3	B	402	YBO	C17-N16	-4.14	1.34	1.40
2	A	401	NAI	C2B-C1B	4.13	1.66	1.53
2	A	401	NAI	O4B-C4B	4.04	1.54	1.45
2	A	401	NAI	C6A-N6A	4.02	1.44	1.34
2	B	401	NAI	C5B-C4B	-4.02	1.39	1.51
2	B	401	NAI	C6A-N6A	3.93	1.44	1.34
2	A	401	NAI	C5B-C4B	-3.91	1.39	1.51
2	A	401	NAI	PN-O3	3.88	1.63	1.59
3	A	402	YBO	S02-N01	3.81	1.67	1.60
2	B	401	NAI	C3B-C4B	3.56	1.62	1.53
3	A	402	YBO	C17-N16	-3.52	1.35	1.40
2	B	401	NAI	O3B-C3B	3.47	1.51	1.43
3	B	402	YBO	C09-C10	3.43	1.56	1.51
3	B	402	YBO	C27-C26	-3.40	1.43	1.48
2	A	401	NAI	C3B-C4B	3.35	1.61	1.53
3	A	402	YBO	C09-C10	3.19	1.55	1.51
3	A	402	YBO	O03-S02	3.15	1.49	1.43
3	A	402	YBO	O22-C20	3.13	1.30	1.22
3	A	402	YBO	C05-S02	3.12	1.81	1.77
2	A	401	NAI	O3D-C3D	3.08	1.50	1.43
2	B	401	NAI	C7N-N7N	3.07	1.42	1.33
2	A	401	NAI	C7N-C3N	3.04	1.55	1.48
3	A	402	YBO	C19-N18	-2.94	1.32	1.38
2	B	401	NAI	O3D-C3D	2.92	1.50	1.43
3	B	402	YBO	C23-C19	2.69	1.41	1.36
3	B	402	YBO	N16-N25	-2.65	1.33	1.38
2	B	401	NAI	O4B-C4B	2.64	1.50	1.45
2	B	401	NAI	C6N-N1N	2.63	1.43	1.37
3	B	402	YBO	C05-S02	2.61	1.80	1.77
2	B	401	NAI	C7N-C3N	2.60	1.54	1.48
3	B	402	YBO	O03-S02	2.58	1.48	1.43
2	A	401	NAI	C8A-N9A	-2.57	1.33	1.37
2	B	401	NAI	C8A-N9A	-2.49	1.33	1.37
3	A	402	YBO	C06-C05	-2.48	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	YBO	C19-N18	-2.45	1.33	1.38
3	B	402	YBO	C09-C08	2.39	1.55	1.51
2	A	401	NAI	C5A-N7A	-2.35	1.34	1.39
2	A	401	NAI	O3B-C3B	2.34	1.48	1.43
3	B	402	YBO	O21-C20	-2.31	1.24	1.30
2	A	401	NAI	C6N-N1N	2.16	1.42	1.37
3	B	402	YBO	C11-N16	-2.15	1.34	1.37
2	B	401	NAI	PN-O5D	2.06	1.67	1.59
2	B	401	NAI	C5A-N7A	-2.06	1.35	1.39

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	YBO	C34-C35-C05	-7.98	118.93	122.66
3	B	402	YBO	O04-S02-O03	-7.61	107.09	118.80
3	A	402	YBO	S24-C17-N18	-7.10	107.48	116.28
3	B	402	YBO	C06-C05-C35	5.75	122.28	118.53
2	B	401	NAI	N3A-C2A-N1A	-5.72	119.93	128.58
3	B	402	YBO	O03-S02-N01	5.27	114.95	107.35
3	B	402	YBO	C26-N25-N16	5.02	109.33	103.97
3	A	402	YBO	O04-S02-O03	-4.99	111.12	118.80
3	A	402	YBO	C26-N25-N16	4.93	109.23	103.97
3	A	402	YBO	C14-C13-C12	-4.74	107.96	120.01
3	B	402	YBO	S24-C17-N18	-4.62	110.56	116.28
2	B	401	NAI	C3N-C2N-N1N	-4.58	116.49	123.20
2	A	401	NAI	N3A-C2A-N1A	-4.42	121.89	128.58
3	A	402	YBO	C17-N18-C19	4.13	116.66	106.79
3	A	402	YBO	O03-S02-N01	4.02	113.16	107.35
2	A	401	NAI	C4A-C5A-N7A	-3.97	106.04	110.58
3	B	402	YBO	C35-C05-S02	-3.87	118.73	121.21
2	B	401	NAI	C6N-N1N-C2N	3.86	123.45	119.32
3	A	402	YBO	C10-C26-N25	-3.78	107.57	111.96
3	B	402	YBO	C15-C13-C12	-3.68	110.65	120.01
2	B	401	NAI	C4D-O4D-C1D	-3.60	101.52	109.47
3	B	402	YBO	C17-N16-N25	3.51	124.57	117.33
2	A	401	NAI	O4B-C1B-N9A	3.43	114.68	108.09
2	A	401	NAI	C1D-N1N-C2N	-3.40	115.54	121.14
2	A	401	NAI	C5A-N7A-C8A	3.38	108.77	103.45
2	A	401	NAI	C5A-C4A-N3A	-3.29	122.18	126.72
2	A	401	NAI	C4D-O4D-C1D	-3.29	102.19	109.47
3	A	402	YBO	C06-C05-C35	3.28	120.67	118.53
2	B	401	NAI	C4A-C5A-N7A	-3.22	106.89	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAI	C3D-C2D-C1D	-3.20	95.41	101.46
3	A	402	YBO	C28-C27-C26	-3.19	115.51	120.74
2	A	401	NAI	C4B-O4B-C1B	-3.17	102.47	109.47
3	B	402	YBO	C19-C23-S24	-3.11	106.65	110.24
3	B	402	YBO	C10-C26-N25	-3.10	108.35	111.96
2	B	401	NAI	C2A-N3A-C4A	3.09	119.39	111.83
2	B	401	NAI	C1D-N1N-C2N	-3.09	116.05	121.14
3	B	402	YBO	F36-C35-C05	3.08	121.30	118.91
2	B	401	NAI	C5A-C4A-N3A	-3.05	122.52	126.72
3	B	402	YBO	O21-C20-C19	3.03	118.27	113.40
2	B	401	NAI	O3-PA-O1A	-3.02	101.62	110.70
2	B	401	NAI	C2A-N1A-C6A	3.02	123.69	118.73
3	B	402	YBO	C11-N16-N25	-3.00	108.34	112.19
2	A	401	NAI	O2A-PA-O3	-2.99	99.20	107.27
2	A	401	NAI	N9A-C8A-N7A	-2.97	109.72	113.94
2	B	401	NAI	C6A-C5A-N7A	2.90	137.68	132.09
3	B	402	YBO	C33-C27-C26	-2.88	116.02	120.74
2	A	401	NAI	C3D-C2D-C1D	-2.84	96.10	101.46
2	B	401	NAI	C2D-C3D-C4D	2.83	108.08	102.61
2	B	401	NAI	O2B-C2B-C3B	2.83	120.88	111.82
3	A	402	YBO	C19-C23-S24	-2.80	107.01	110.24
3	A	402	YBO	C11-N16-N25	-2.79	108.61	112.19
2	B	401	NAI	O4B-C1B-N9A	2.75	113.38	108.09
2	B	401	NAI	C5A-N7A-C8A	2.70	107.70	103.45
3	B	402	YBO	C17-N18-C19	2.65	113.11	106.79
2	A	401	NAI	C2A-N1A-C6A	2.64	123.07	118.73
3	A	402	YBO	O22-C20-C19	-2.64	117.85	122.02
3	B	402	YBO	C23-C19-C20	-2.63	119.19	124.28
3	A	402	YBO	C17-N16-N25	2.59	122.68	117.33
2	A	401	NAI	O4B-C1B-C2B	-2.59	101.07	106.62
2	A	401	NAI	O2B-C2B-C3B	2.55	119.98	111.82
2	B	401	NAI	N9A-C8A-N7A	-2.53	110.34	113.94
2	A	401	NAI	C2A-N3A-C4A	2.51	117.97	111.83
2	B	401	NAI	O3B-C3B-C2B	2.51	119.85	111.82
3	B	402	YBO	C33-C32-C30	2.45	120.90	118.38
3	B	402	YBO	C13-C12-C11	-2.43	108.51	113.86
2	B	401	NAI	O1N-PN-O3	2.32	113.56	107.27
3	B	402	YBO	C05-S02-N01	2.32	112.45	108.28
2	B	401	NAI	O2B-C2B-C1B	-2.31	102.15	110.10
2	A	401	NAI	C6A-C5A-N7A	2.27	136.47	132.09
3	A	402	YBO	C32-C30-C29	-2.22	119.88	122.80
3	B	402	YBO	C32-C33-C27	-2.22	118.43	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAI	C4A-N9A-C1B	-2.18	121.52	126.63
2	A	401	NAI	O4D-C4D-C5D	-2.12	102.54	109.33
2	B	401	NAI	O4B-C1B-C2B	-2.12	102.08	106.62
3	A	402	YBO	O04-S02-C05	2.07	110.27	107.26
3	A	402	YBO	C34-C35-C05	-2.05	121.70	122.66
3	B	402	YBO	C10-C11-N16	2.05	109.54	107.08
3	B	402	YBO	O22-C20-C19	-2.04	118.80	122.02
2	B	401	NAI	C3B-C2B-C1B	2.03	105.30	101.46

There are no chirality outliers.

All (25) torsion outliers are listed below:

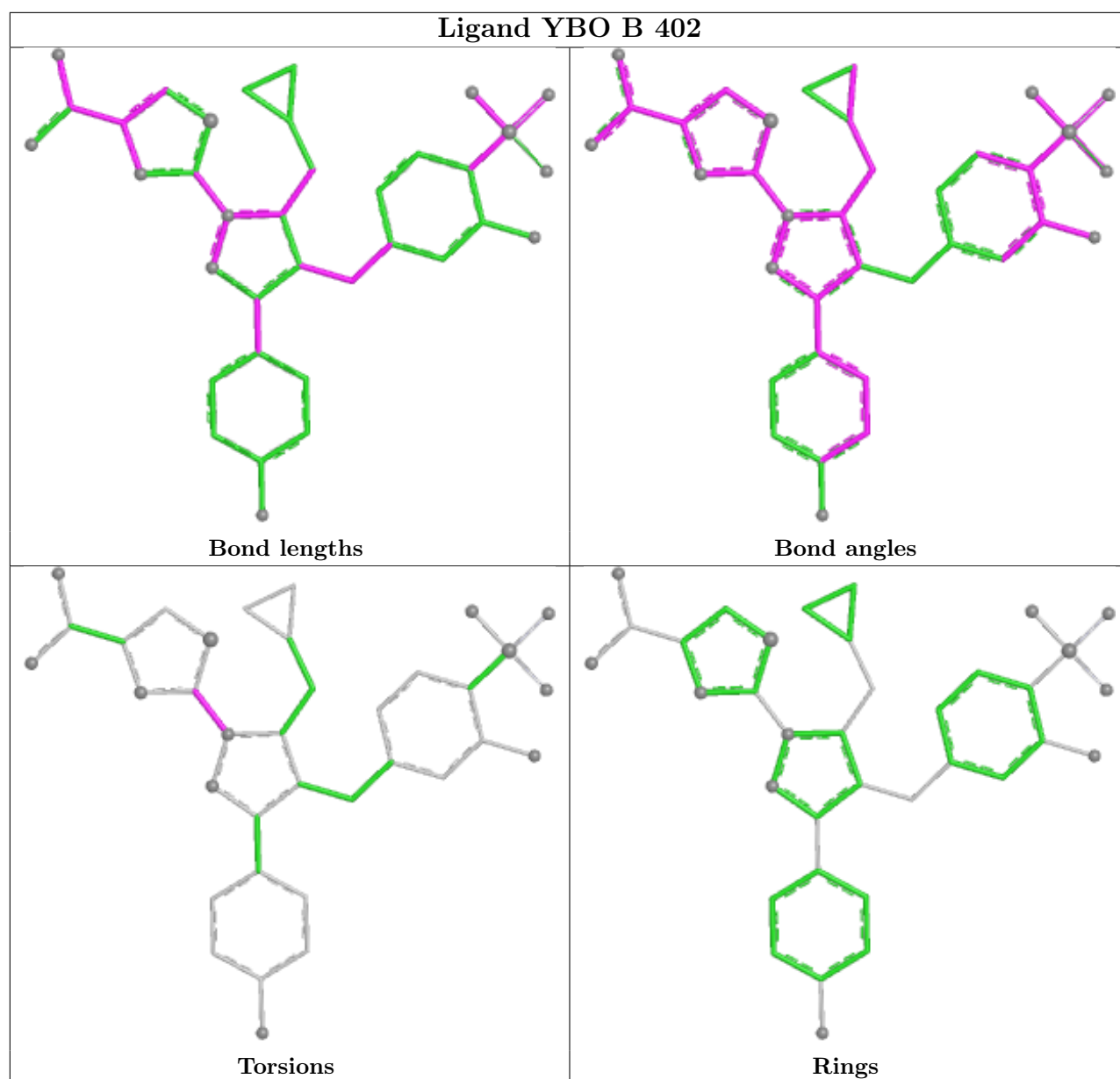
Mol	Chain	Res	Type	Atoms
5	B	403	PEG	O1-C1-C2-O2
5	B	403	PEG	O2-C3-C4-O4
4	A	408	EDO	O1-C1-C2-O2
4	A	405	EDO	O1-C1-C2-O2
4	A	407	EDO	O1-C1-C2-O2
4	B	408	EDO	O1-C1-C2-O2
4	A	404	EDO	O1-C1-C2-O2
4	B	405	EDO	O1-C1-C2-O2
2	B	401	NAI	C2D-C1D-N1N-C2N
4	A	406	EDO	O1-C1-C2-O2
4	A	412	EDO	O1-C1-C2-O2
5	B	403	PEG	C4-C3-O2-C2
2	B	401	NAI	O4D-C1D-N1N-C2N
4	B	404	EDO	O1-C1-C2-O2
4	B	407	EDO	O1-C1-C2-O2
2	A	401	NAI	O4D-C1D-N1N-C2N
4	A	411	EDO	O1-C1-C2-O2
2	A	401	NAI	C2D-C1D-N1N-C2N
2	B	401	NAI	O4D-C1D-N1N-C6N
4	B	406	EDO	O1-C1-C2-O2
2	B	401	NAI	C2D-C1D-N1N-C6N
4	A	410	EDO	O1-C1-C2-O2
2	A	401	NAI	O4B-C4B-C5B-O5B
3	A	402	YBO	N18-C17-N16-N25
3	B	402	YBO	N18-C17-N16-N25

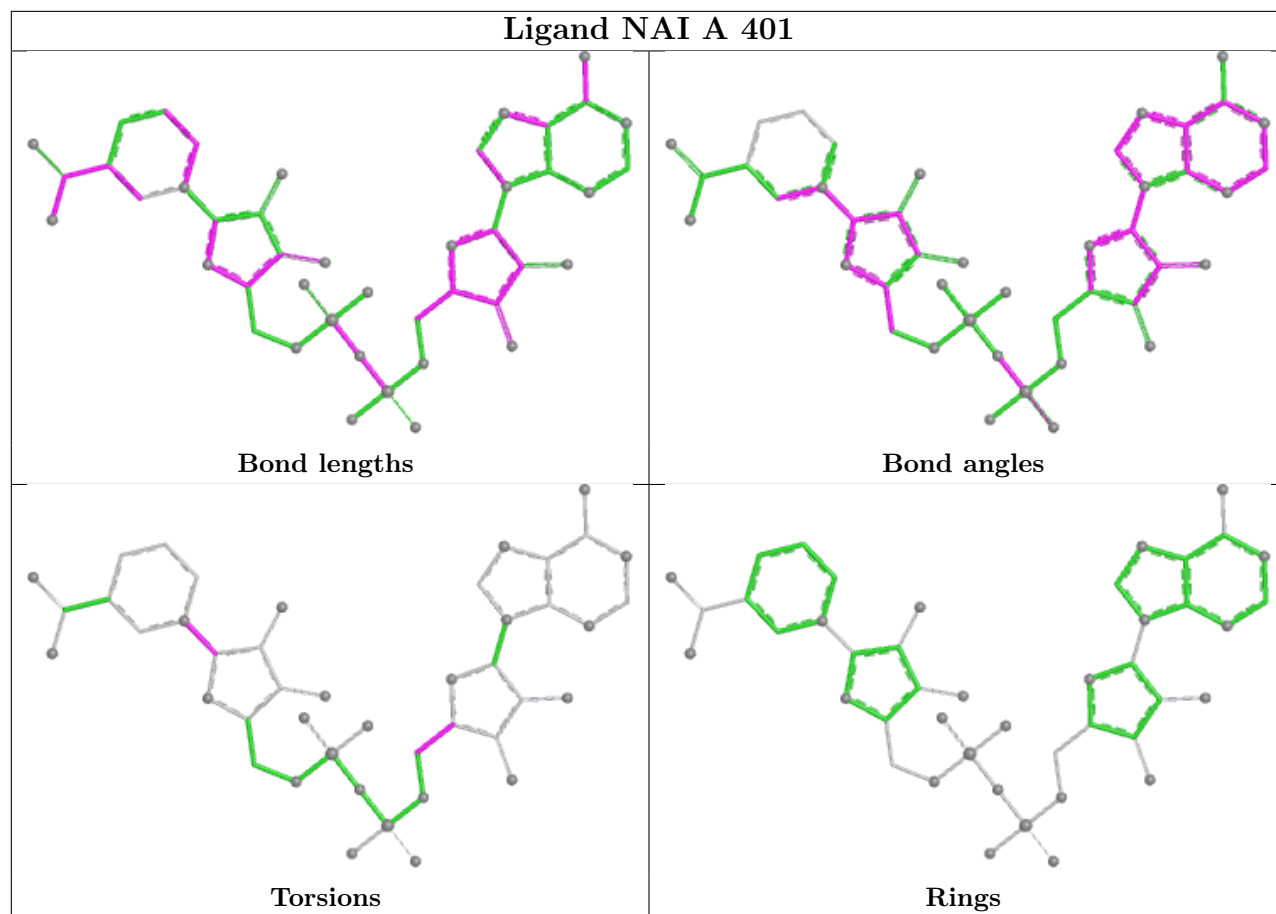
There are no ring outliers.

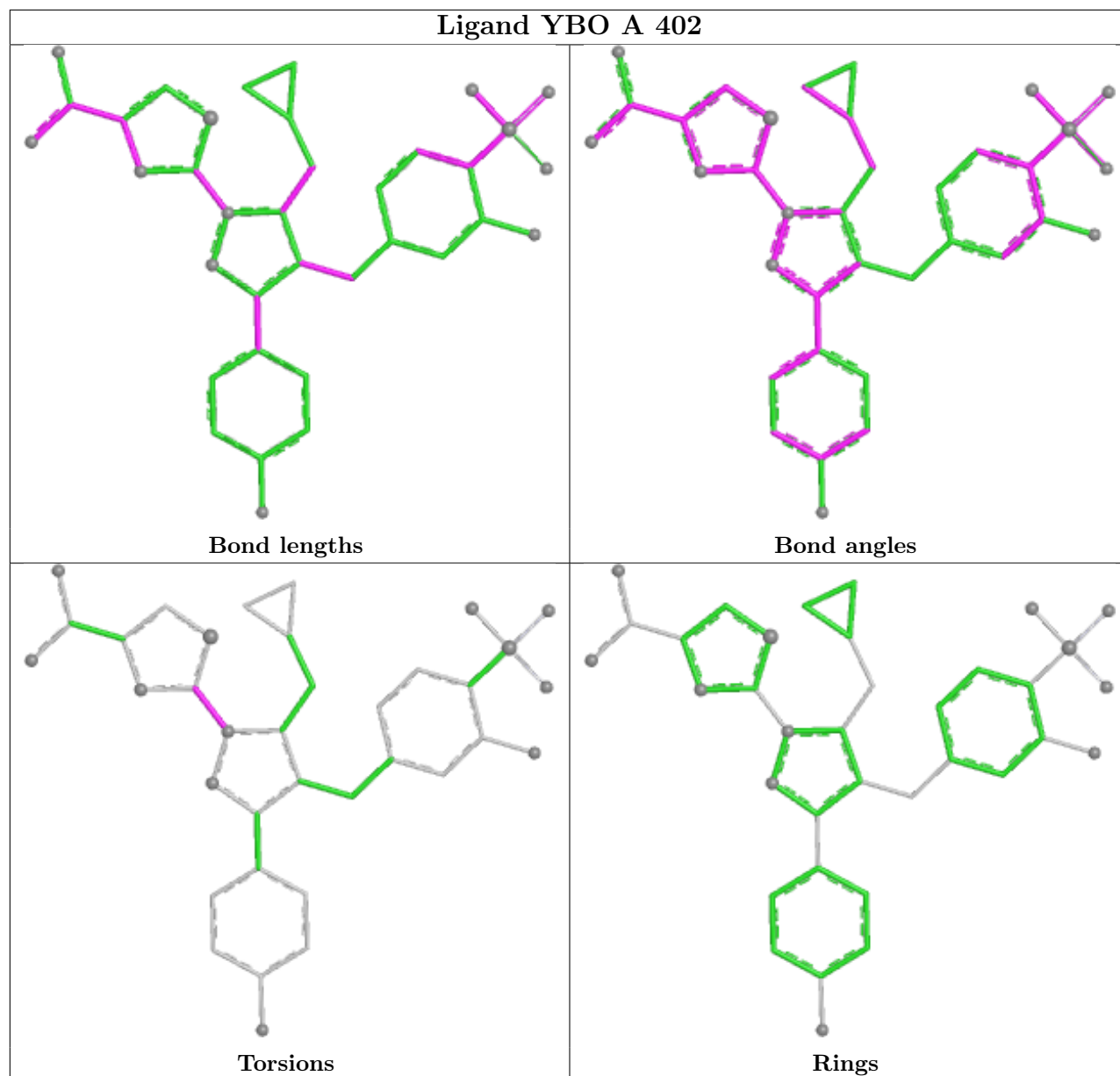
9 monomers are involved in 15 short contacts:

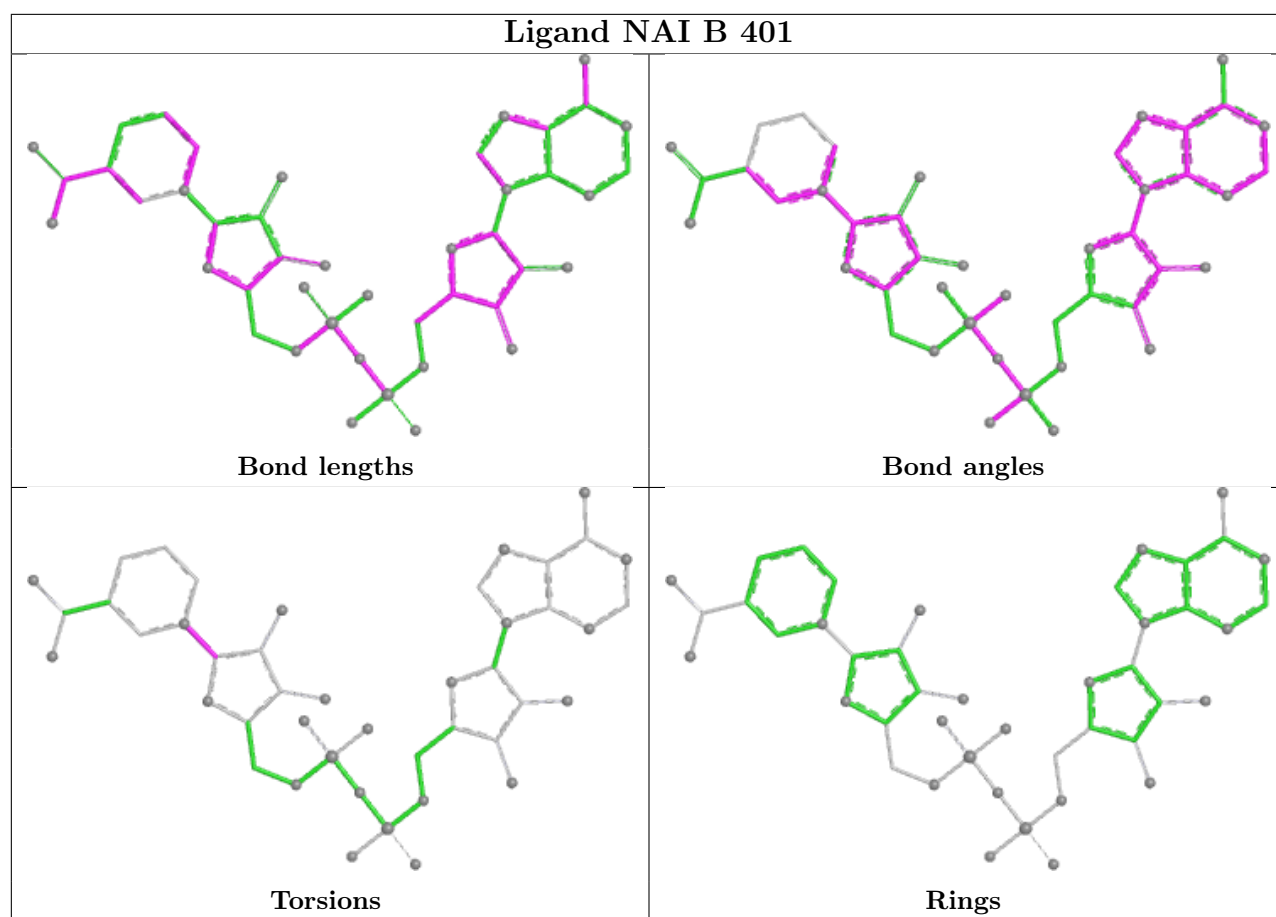
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	409	EDO	1	0
3	B	402	YBO	1	0
2	A	401	NAI	4	0
4	B	404	EDO	3	0
3	A	402	YBO	2	0
2	B	401	NAI	2	0
4	B	406	EDO	3	0
4	A	407	EDO	1	0
4	B	405	EDO	1	0

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.









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	331/338 (97%)	-0.44	3 (0%)	81 84	17, 29, 49, 106	1 (0%)
1	B	331/338 (97%)	-0.25	5 (1%)	72 76	18, 34, 59, 106	1 (0%)
All	All	662/676 (97%)	-0.35	8 (1%)	76 80	17, 32, 57, 106	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	332	PHE	4.8
1	A	332	PHE	3.9
1	B	2	ALA	3.4
1	A	2	ALA	2.5
1	B	12	LEU	2.5
1	A	18	THR	2.4
1	B	330	LEU	2.1
1	B	280	LEU	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,

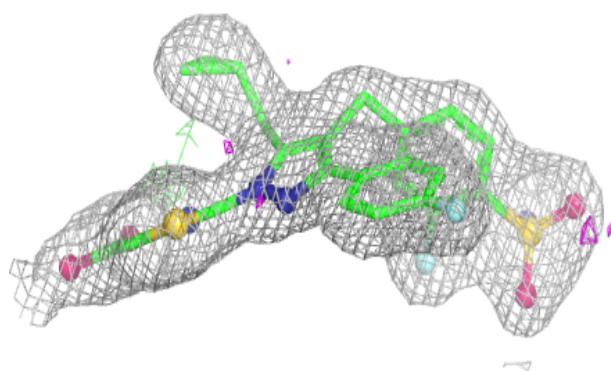
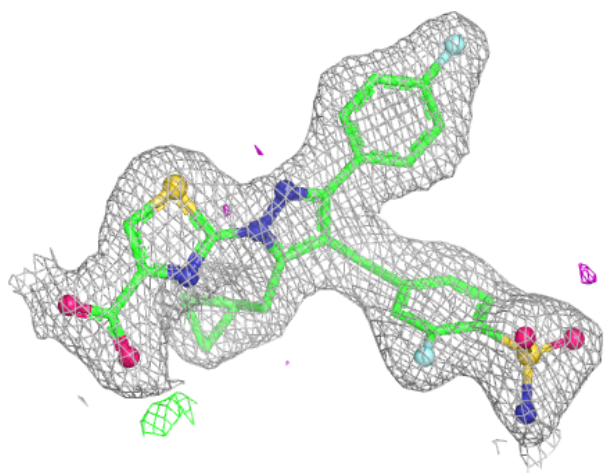
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	411	4/4	0.79	0.18	43,43,47,48	0
4	EDO	A	413	4/4	0.81	0.14	64,65,65,72	0
4	EDO	A	409	4/4	0.82	0.18	55,55,58,58	0
4	EDO	A	405	4/4	0.84	0.15	56,67,69,80	0
4	EDO	A	408	4/4	0.85	0.18	61,64,67,68	0
4	EDO	A	412	4/4	0.86	0.14	53,60,66,74	0
4	EDO	A	403	4/4	0.86	0.14	48,51,51,56	0
5	PEG	B	403	7/7	0.86	0.13	60,62,63,63	0
4	EDO	B	409	4/4	0.87	0.14	52,54,56,59	0
4	EDO	B	406	4/4	0.88	0.15	48,53,54,59	0
4	EDO	B	407	4/4	0.88	0.17	61,63,65,72	0
4	EDO	A	406	4/4	0.88	0.14	59,60,60,65	0
4	EDO	B	405	4/4	0.88	0.14	49,51,57,62	0
4	EDO	B	404	4/4	0.91	0.13	48,51,51,55	0
4	EDO	B	408	4/4	0.91	0.12	59,64,64,70	0
4	EDO	A	404	4/4	0.92	0.10	50,58,59,65	0
4	EDO	A	410	4/4	0.92	0.12	39,46,47,47	0
4	EDO	A	407	4/4	0.94	0.17	39,44,46,50	0
3	YBO	A	402	36/36	0.98	0.05	22,27,30,31	0
3	YBO	B	402	36/36	0.98	0.06	27,32,37,44	0
2	NAI	A	401	44/44	0.98	0.04	23,27,29,30	0
2	NAI	B	401	44/44	0.98	0.05	28,33,38,39	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.

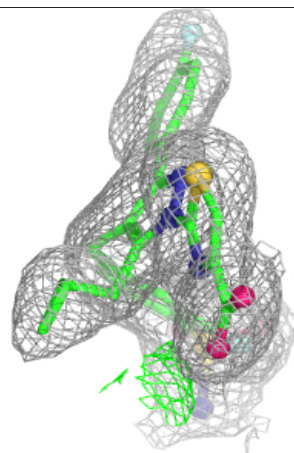
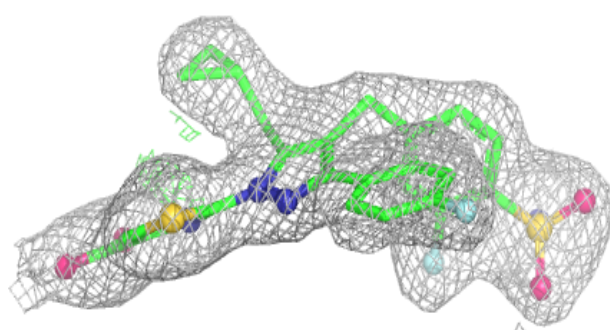
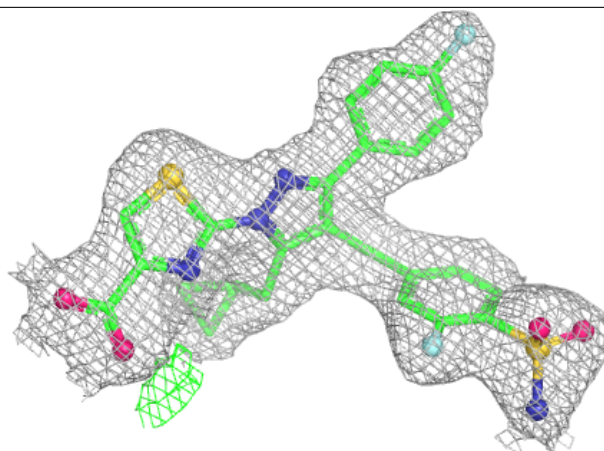
Electron density around YBO A 402:

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

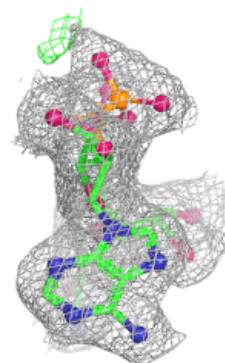
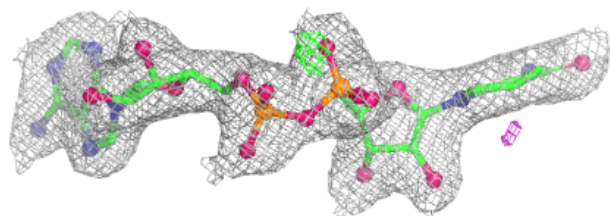
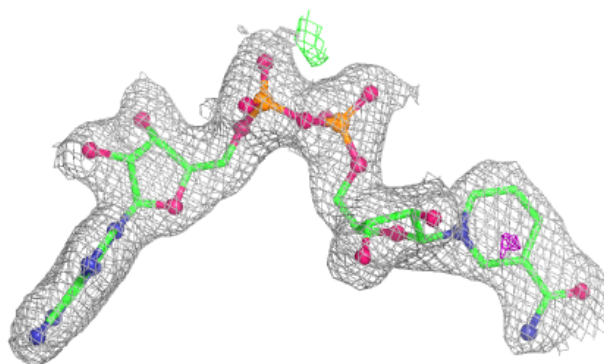


Electron density around YBO B 402:

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

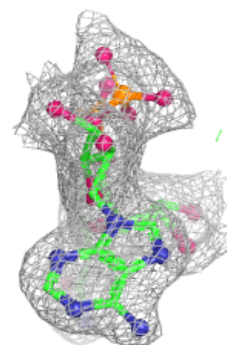
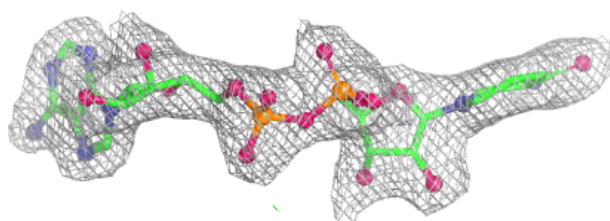
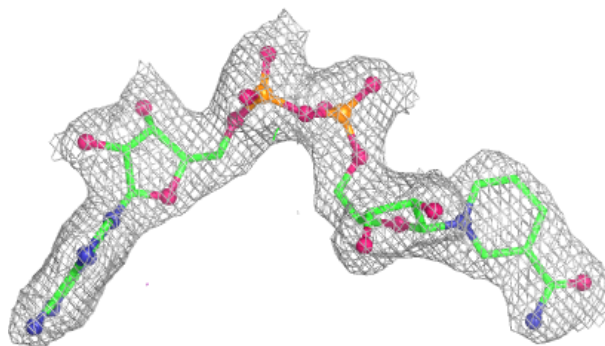
**Electron density around NAI A 401:**

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



Electron density around NAI 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.