



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:47 PM UTC

PDB ID : 7WAS / pdb_00007was
Title : SbSOMT in complex with pterostilbene and nicotinamide adenine dinucleotide(NAD+)
Authors : Pow, K.C.; Hao, Q.
Deposited on : 2021-12-14
Resolution : 2.40 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

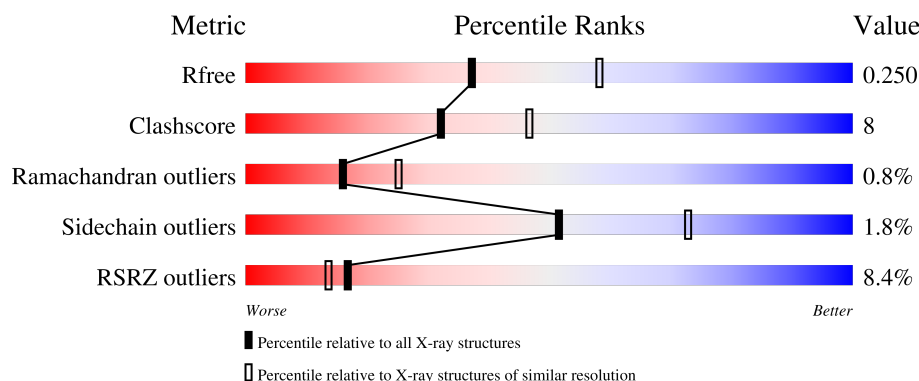
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	376	10% 81% 13% ...
1	B	376	6% 78% 16% ...

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	407	-	-	X	-

2 Entry composition [i](#)

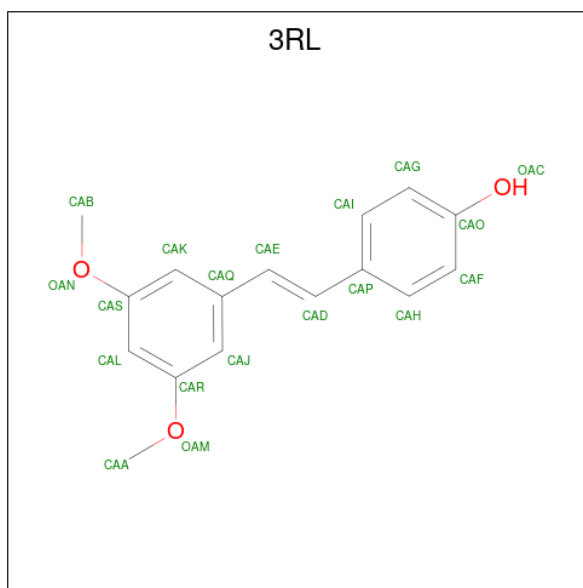
There are 8 unique types of molecules in this entry. The entry contains 6104 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 stilbene O-methyltransferase.

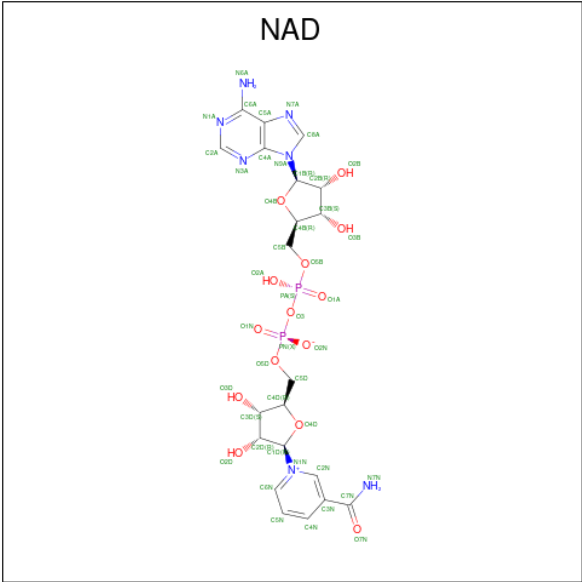
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	6	0
			2861	1822	478	538	23			
1	B	363	Total	C	N	O	S	0	6	0
			2860	1822	478	536	24			

- Molecule 2 is Pterostilbene (CCD ID: 3RL) (formula: C₁₆H₁₆O₃) (labeled as "Ligand of Interest" by depositor).



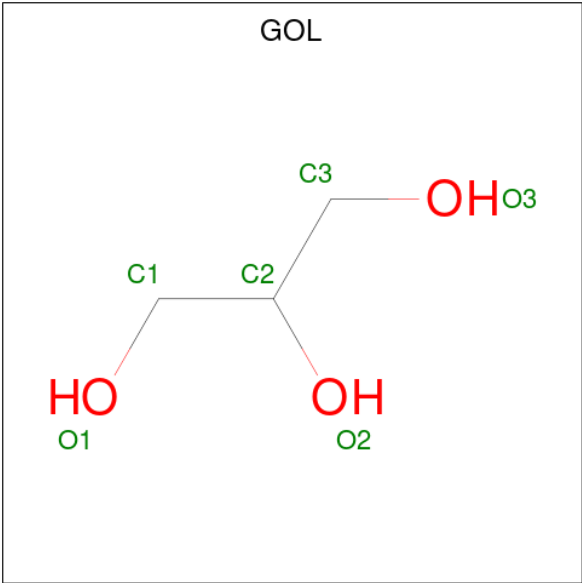
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	16	3		
2	B	1	Total	C	O	0	0
			19	16	3		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



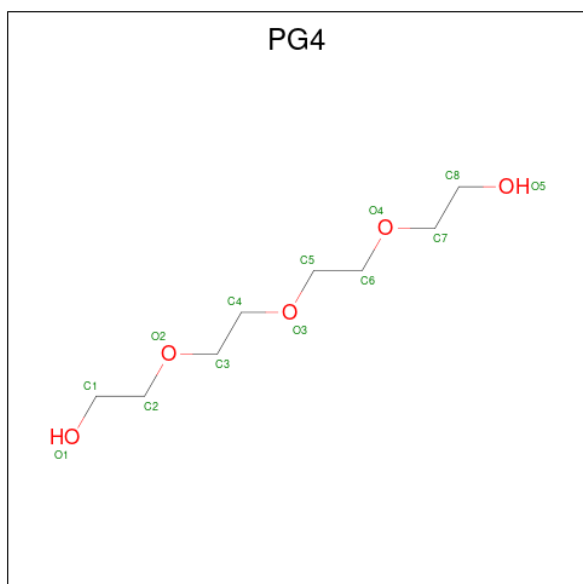
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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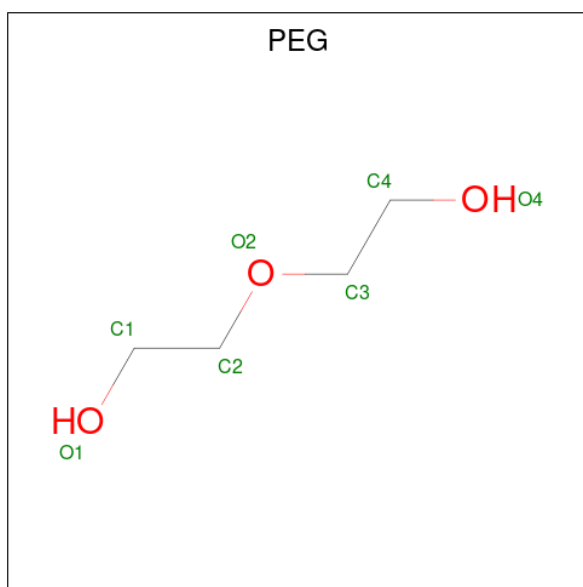
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



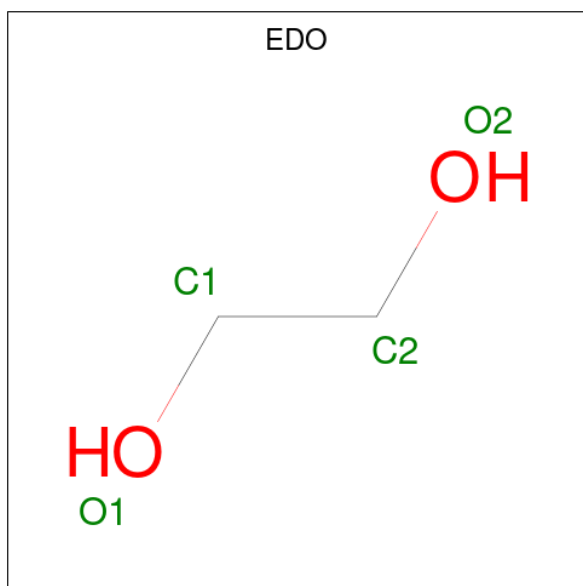
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

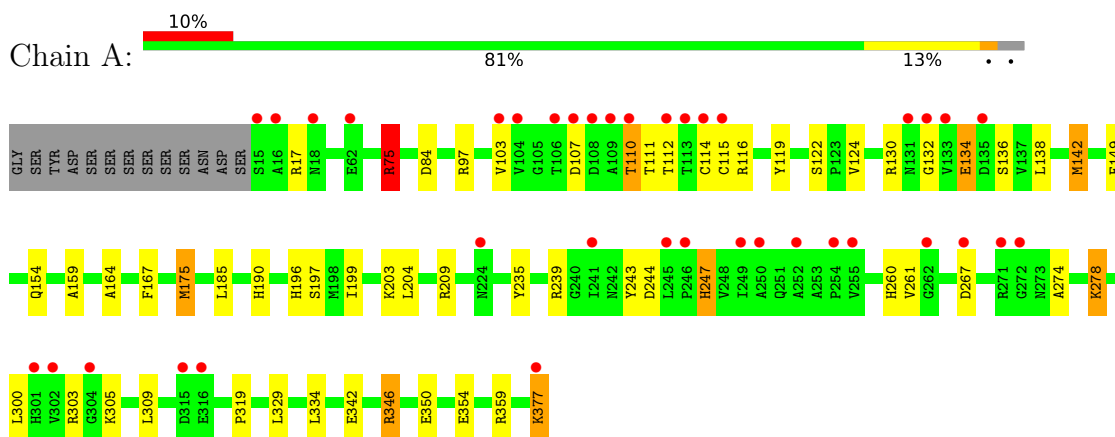
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	79	Total	O	0	0
			79	79		
8	B	90	Total	O	0	0
			90	90		

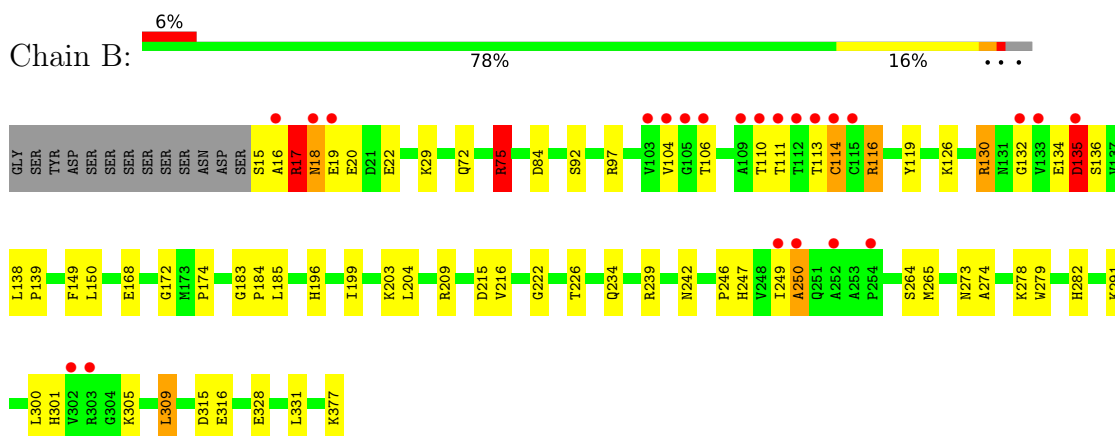
3 Residue-property plots [i](#)

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: stilbene O-methyltransferase



- Molecule 1: stilbene O-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.47Å 96.47Å 169.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.42 – 2.40 31.42 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (31.42-2.40) 99.1 (31.42-2.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.187 , 0.246 0.194 , 0.250	Depositor DCC
R_{free} test set	1899 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6104	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: PG4, EDO, GOL, NAD, PEG, 3RL

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	0.98	5/2919 (0.2%)	1.37	7/3957 (0.2%)
1	B	1.01	4/2918 (0.1%)	1.33	4/3955 (0.1%)
All	All	0.99	9/5837 (0.2%)	1.35	11/7912 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	7
All	All	0	13

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	301	HIS	CE1-NE2	9.69	1.42	1.32
1	A	260	HIS	CE1-NE2	7.66	1.40	1.32
1	A	196	HIS	CE1-NE2	7.64	1.40	1.32
1	B	196	HIS	CE1-NE2	7.53	1.40	1.32
1	B	282	HIS	CE1-NE2	7.52	1.40	1.32
1	A	142	MET	CG-SD	6.38	1.96	1.80
1	A	190	HIS	CE1-NE2	6.38	1.39	1.32
1	B	247	HIS	CE1-NE2	6.34	1.38	1.32
1	A	175	MET	CG-SD	-5.48	1.67	1.80

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	THR	CA-CB-OG1	7.97	121.56	109.60
1	B	135	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	267	ASP	O-C-N	5.96	129.17	122.32
1	A	110	THR	CB-CA-C	5.72	120.75	109.66
1	A	235	TYR	CA-C-N	5.53	127.95	120.38
1	A	235	TYR	C-N-CA	5.53	127.95	120.38
1	A	377	LYS	CA-C-O	-5.24	111.89	120.80
1	B	29	LYS	O-C-N	-5.19	116.69	122.09
1	B	75	ARG	N-CA-CB	-5.17	103.61	111.21
1	A	247	HIS	CA-CB-CG	5.17	118.97	113.80
1	B	226	THR	CA-CB-CG2	5.04	119.07	110.50

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	239	ARG	Sidechain
1	A	303	ARG	Sidechain
1	A	346	ARG	Sidechain
1	A	359	ARG	Sidechain
1	A	75	ARG	Sidechain
1	B	114	CYS	Peptide
1	B	116	ARG	Sidechain
1	B	130	ARG	Sidechain
1	B	132	GLY	Peptide
1	B	17	ARG	Sidechain
1	B	209	ARG	Sidechain
1	B	75	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2861	0	2832	34	0
1	B	2860	0	2835	60	0
2	A	19	0	16	0	0
2	B	19	0	16	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	44	0	26	1	0
3	B	44	0	26	8	0
4	A	12	0	16	0	0
4	B	36	0	48	9	0
5	A	13	0	18	3	0
6	A	7	0	10	3	0
7	A	8	0	12	2	0
7	B	12	0	18	0	0
8	A	79	0	0	3	0
8	B	90	0	0	10	0
All	All	6104	0	5873	94	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 8.

All (94) 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:291:LYS:HD2	3:B:403:NAD:H5N	1.43	0.97
1:A:17:ARG:NH1	6:A:406:PEG:H12	1.78	0.97
1:A:124:VAL:HB	5:A:405:PG4:H71	1.51	0.90
1:B:17:ARG:O	1:B:19:GLU:N	2.04	0.90
1:B:291:LYS:CD	3:B:403:NAD:H5N	2.07	0.84
1:A:122:SER:HB3	5:A:405:PG4:H61	1.58	0.83
1:B:246:PRO:O	1:B:249:ILE:O	1.97	0.82
1:B:316[B]:GLU:OE1	8:B:501:HOH:O	1.98	0.80
2:B:402:3RL:OAC	4:B:407:GOL:H12	1.81	0.80
1:B:126:LYS:NZ	8:B:503:HOH:O	2.20	0.74
1:B:264:SER:OG	3:B:403:NAD:H52A	1.92	0.69
1:B:249:ILE:O	1:B:250:ALA:HB2	1.96	0.66
1:B:110:THR:CG2	8:B:558:HOH:O	2.43	0.65
1:B:106:THR:HG23	1:B:113:THR:HG22	1.79	0.65
1:B:106:THR:HG23	1:B:113:THR:CG2	2.28	0.63
1:A:130:ARG:HG2	1:A:138:LEU:CD2	2.30	0.61
1:B:328:GLU:CD	4:B:407:GOL:H32	2.25	0.60
1:A:142:MET:HE3	8:A:526:HOH:O	2.02	0.59
1:B:315[A]:ASP:O	1:B:316[A]:GLU:HG3	2.01	0.59
1:A:154:GLN:HE22	1:B:150:LEU:HD12	1.68	0.59
1:B:215:ASP:HB2	1:B:273:ASN:OD1	2.03	0.58
1:A:84:ASP:OD2	1:A:111:THR:HG22	2.05	0.57
1:A:300:LEU:O	1:A:377:LYS:NZ	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LYS:HD3	1:B:279:TRP:HB2	1.86	0.56
1:B:291:LYS:HD2	3:B:403:NAD:C5N	2.26	0.55
1:B:17:ARG:C	1:B:19:GLU:N	2.65	0.55
1:B:249:ILE:O	1:B:250:ALA:CB	2.53	0.55
1:B:15:SER:C	1:B:17:ARG:H	2.15	0.55
1:B:300:LEU:O	1:B:377:LYS:NZ	2.34	0.54
1:B:199:ILE:O	1:B:203:LYS:HG2	2.08	0.54
1:A:247:HIS:HB3	7:A:407:EDO:C1	2.38	0.54
1:B:84:ASP:OD2	1:B:111:THR:HG22	2.08	0.53
1:B:265:MET:H	3:B:403:NAD:C2A	2.21	0.53
1:A:114:CYS:C	1:A:115:CYS:SG	2.92	0.53
1:B:222:GLY:HA3	1:B:242:ASN:OD1	2.09	0.51
1:A:197:SER:OG	1:A:278:LYS:NZ	2.25	0.51
1:B:135:ASP:OD2	8:B:502:HOH:O	2.19	0.51
2:B:402:3RL:OAC	4:B:407:GOL:C1	2.57	0.51
1:A:199:ILE:O	1:A:203:LYS:HG2	2.11	0.51
1:B:15:SER:OG	1:B:22:GLU:HG3	2.11	0.51
1:A:350:GLU:O	1:A:354:GLU:HG2	2.11	0.50
1:B:168[A]:GLU:OE2	4:B:409:GOL:O1	2.27	0.50
1:B:110:THR:HG22	8:B:558:HOH:O	2.07	0.49
1:B:130:ARG:HG2	1:B:138:LEU:HD22	1.93	0.49
1:B:328:GLU:CD	4:B:407:GOL:C3	2.87	0.48
1:B:279:TRP:CH2	2:B:402:3RL:HAH	2.48	0.48
2:B:402:3RL:CAO	4:B:407:GOL:H12	2.43	0.48
1:A:209:ARG:HD3	8:A:577:HOH:O	2.14	0.48
1:A:334:LEU:HD23	1:A:334:LEU:C	2.39	0.48
1:B:264:SER:HA	3:B:403:NAD:H2A	1.94	0.48
1:B:110:THR:HB	8:B:558:HOH:O	2.14	0.48
1:A:17:ARG:HH11	6:A:406:PEG:H12	1.73	0.48
1:A:110:THR:HG23	1:A:112:THR:O	2.14	0.48
1:B:138:LEU:HB3	1:B:139:PRO:HD3	1.96	0.47
1:A:103:VAL:HG11	1:A:107:ASP:HB2	1.97	0.47
1:B:15:SER:O	1:B:17:ARG:N	2.38	0.47
1:B:18:ASN:O	1:B:19:GLU:HB3	2.14	0.47
1:A:97:ARG:O	1:A:119:TYR:HA	2.14	0.46
1:B:15:SER:C	1:B:17:ARG:N	2.73	0.46
1:B:75:ARG:HG2	1:B:75:ARG:HH11	1.81	0.46
1:B:328:GLU:OE1	4:B:407:GOL:H32	2.16	0.46
1:A:111:THR:O	1:A:111:THR:OG1	2.32	0.45
1:B:279:TRP:CE3	2:B:402:3RL:HAM	2.53	0.44
1:B:18:ASN:C	1:B:20:GLU:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:PHE:CE2	1:B:185:LEU:HD11	2.52	0.44
1:B:97:ARG:HA	4:B:404:GOL:H12	2.00	0.44
1:B:116:ARG:HD2	8:B:571:HOH:O	2.17	0.44
1:B:97:ARG:O	1:B:119:TYR:HA	2.18	0.43
1:B:234:GLN:HB2	8:B:540:HOH:O	2.17	0.43
1:A:247:HIS:HB3	7:A:407:EDO:C2	2.48	0.43
1:B:110:THR:CB	8:B:558:HOH:O	2.65	0.43
1:B:291:LYS:NZ	3:B:403:NAD:H5N	2.33	0.43
1:B:183:GLY:N	1:B:184:PRO:CD	2.81	0.43
1:A:244:ASP:HA	3:A:402:NAD:N1A	2.33	0.43
1:A:319:PRO:HA	1:B:92:SER:O	2.19	0.42
1:B:216:VAL:HA	1:B:239:ARG:O	2.19	0.42
1:A:159:ALA:HB1	1:A:164:ALA:O	2.18	0.42
1:A:204:LEU:HD22	1:A:309:LEU:HD21	2.01	0.42
1:A:97:ARG:HH12	5:A:405:PG4:H41	1.85	0.42
1:B:204:LEU:HD22	1:B:309:LEU:HD21	2.01	0.42
1:B:15:SER:N	8:B:518:HOH:O	2.53	0.41
1:B:18:ASN:O	1:B:19:GLU:CB	2.67	0.41
1:A:346:ARG:CZ	1:B:114:CYS:HB3	2.51	0.41
1:B:265:MET:N	3:B:403:NAD:H2A	2.36	0.41
1:A:167:PHE:CE1	1:A:175:MET:HA	2.55	0.41
1:A:243:TYR:HA	1:A:261:VAL:O	2.21	0.41
1:A:274:ALA:HA	1:A:305:LYS:O	2.20	0.41
1:B:274:ALA:HA	1:B:305:LYS:O	2.21	0.41
1:A:75:ARG:NH2	8:A:512:HOH:O	2.54	0.41
1:A:329:LEU:HD23	1:A:342:GLU:CD	2.46	0.40
1:B:168[B]:GLU:HG2	1:B:174:PRO:HA	2.04	0.40
1:A:17:ARG:HH12	6:A:406:PEG:H12	1.73	0.40
1:A:149:PHE:CE2	1:A:185:LEU:HD11	2.56	0.40
1:B:172:GLY:O	4:B:409:GOL:O2	2.33	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	367/376 (98%)	348 (95%)	17 (5%)	2 (0%)	24	37
1	B	367/376 (98%)	353 (96%)	10 (3%)	4 (1%)	11	18
All	All	734/752 (98%)	701 (96%)	27 (4%)	6 (1%)	16	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	GLU
1	B	16	ALA
1	B	18	ASN
1	B	250	ALA
1	B	104	VAL
1	A	132	GLY

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	306/312 (98%)	302 (99%)	4 (1%)	61	80
1	B	306/312 (98%)	299 (98%)	7 (2%)	44	66
All	All	612/624 (98%)	601 (98%)	11 (2%)	51	73

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

Mol	Chain	Res	Type
1	A	75	ARG
1	A	134	GLU
1	A	136	SER
1	A	278	LYS
1	B	17	ARG
1	B	72	GLN
1	B	134	GLU

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Mol	Chain	Res	Type
1	B	135	ASP
1	B	136	SER
1	B	309	LEU
1	B	331	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	234	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](#)

19 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	$\# Z > 2$
4	GOL	B	401	-	5,5,5	0.32	0	5,5,5	1.17	0
7	EDO	B	411	-	3,3,3	0.20	0	2,2,2	0.10	0
7	EDO	A	408	-	3,3,3	0.72	0	2,2,2	0.81	0
4	GOL	B	408	-	5,5,5	0.15	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	3RL	B	402	-	20,20,20	0.69	0	26,26,26	0.64	0
5	PG4	A	405	-	12,12,12	0.27	0	11,11,11	0.52	0
7	EDO	B	406	-	3,3,3	0.37	0	2,2,2	0.75	0
4	GOL	B	410	-	5,5,5	0.29	0	5,5,5	0.58	0
4	GOL	A	403	-	5,5,5	0.46	0	5,5,5	0.83	0
6	PEG	A	406	-	6,6,6	0.66	0	5,5,5	0.38	0
4	GOL	B	409	-	5,5,5	0.42	0	5,5,5	0.97	0
7	EDO	B	405	-	3,3,3	0.15	0	2,2,2	0.10	0
4	GOL	B	407	-	5,5,5	0.50	0	5,5,5	1.03	0
2	3RL	A	401	-	20,20,20	0.70	0	26,26,26	0.55	0
3	NAD	B	403	-	46,48,48	1.16	4 (8%)	64,73,73	1.32	7 (10%)
4	GOL	A	404	-	5,5,5	0.35	0	5,5,5	0.62	0
4	GOL	B	404	-	5,5,5	0.23	0	5,5,5	0.40	0
3	NAD	A	402	-	46,48,48	0.91	4 (8%)	64,73,73	1.12	6 (9%)
7	EDO	A	407	-	3,3,3	0.84	0	2,2,2	0.80	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
4	GOL	B	401	-	-	1/4/4/4	-
7	EDO	B	411	-	-	1/1/1/1	-
7	EDO	A	408	-	-	1/1/1/1	-
4	GOL	B	408	-	-	0/4/4/4	-
2	3RL	B	402	-	-	0/9/9/9	0/2/2/2
5	PG4	A	405	-	-	5/10/10/10	-
7	EDO	B	406	-	-	1/1/1/1	-
4	GOL	B	410	-	-	0/4/4/4	-
4	GOL	A	403	-	-	3/4/4/4	-
6	PEG	A	406	-	-	2/4/4/4	-
4	GOL	B	409	-	-	0/4/4/4	-
7	EDO	B	405	-	-	0/1/1/1	-
4	GOL	B	407	-	-	2/4/4/4	-
2	3RL	A	401	-	-	2/9/9/9	0/2/2/2
3	NAD	B	403	-	-	11/30/62/62	0/5/5/5
4	GOL	A	404	-	-	1/4/4/4	-
4	GOL	B	404	-	-	4/4/4/4	-
3	NAD	A	402	-	-	9/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	407	-	-	1/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	NAD	PA-O3	3.80	1.63	1.59
3	B	403	NAD	PN-O3	3.62	1.63	1.59
3	B	403	NAD	C2N-N1N	3.46	1.38	1.35
3	A	402	NAD	PA-O3	2.75	1.62	1.59
3	A	402	NAD	C2N-N1N	2.72	1.38	1.35
3	B	403	NAD	C2A-N1A	-2.38	1.29	1.33
3	A	402	NAD	PN-O3	2.28	1.62	1.59
3	A	402	NAD	O4D-C1D	2.19	1.43	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	NAD	C4D-O4D-C1D	-6.28	104.17	109.92
3	A	402	NAD	C2N-C3N-C7N	-4.31	107.03	119.46
3	A	402	NAD	C4N-C3N-C7N	4.08	132.17	121.06
3	B	403	NAD	C4N-C3N-C7N	-2.69	113.72	121.06
3	B	403	NAD	C2N-C3N-C7N	2.37	126.30	119.46
3	A	402	NAD	C6N-N1N-C1D	2.29	124.22	119.73
3	A	402	NAD	C2N-C3N-C4N	2.18	120.79	118.26
3	B	403	NAD	O3D-C3D-C2D	-2.10	105.08	111.82
3	B	403	NAD	O3D-C3D-C4D	2.08	117.07	111.08
3	B	403	NAD	C6N-N1N-C1D	-2.06	115.69	119.73
3	A	402	NAD	C3N-C7N-N7N	2.03	120.23	117.74
3	B	403	NAD	C2N-N1N-C1D	2.01	123.57	119.13
3	A	402	NAD	O7N-C7N-C3N	-2.01	117.14	119.60

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAD	C5D-O5D-PN-O2N
3	A	402	NAD	O4D-C4D-C5D-O5D
3	A	402	NAD	C2D-C1D-N1N-C2N
3	A	402	NAD	C2D-C1D-N1N-C6N
3	B	403	NAD	C5B-O5B-PA-O1A
3	B	403	NAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	B	403	NAD	C5B-O5B-PA-O3
3	B	403	NAD	O4B-C1B-N9A-C8A
3	B	403	NAD	O4B-C1B-N9A-C4A
4	A	403	GOL	O1-C1-C2-C3
4	B	404	GOL	O1-C1-C2-O2
4	B	404	GOL	C1-C2-C3-O3
4	B	407	GOL	O1-C1-C2-C3
5	A	405	PG4	O3-C5-C6-O4
3	A	402	NAD	C3D-C4D-C5D-O5D
6	A	406	PEG	O2-C3-C4-O4
4	B	401	GOL	C1-C2-C3-O3
4	B	404	GOL	O1-C1-C2-C3
4	A	403	GOL	O1-C1-C2-O2
4	B	404	GOL	O2-C2-C3-O3
7	B	406	EDO	O1-C1-C2-O2
4	B	407	GOL	O1-C1-C2-O2
4	A	404	GOL	O1-C1-C2-O2
7	B	411	EDO	O1-C1-C2-O2
4	A	403	GOL	O2-C2-C3-O3
5	A	405	PG4	C5-C6-O4-C7
7	A	407	EDO	O1-C1-C2-O2
5	A	405	PG4	C1-C2-O2-C3
3	A	402	NAD	PN-O3-PA-O1A
3	A	402	NAD	C4D-C5D-O5D-PN
3	A	402	NAD	C5D-O5D-PN-O3
3	A	402	NAD	C5D-O5D-PN-O1N
3	B	403	NAD	C5D-O5D-PN-O1N
3	B	403	NAD	C4B-C5B-O5B-PA
3	B	403	NAD	C4D-C5D-O5D-PN
2	A	401	3RL	CAE-CAD-CAP-CAI
2	A	401	3RL	CAL-CAR-OAM-CAA
7	A	408	EDO	O1-C1-C2-O2
5	A	405	PG4	C8-C7-O4-C6
3	B	403	NAD	PA-O3-PN-O2N
5	A	405	PG4	O2-C3-C4-O3
6	A	406	PEG	C1-C2-O2-C3
3	B	403	NAD	PA-O3-PN-O1N
3	B	403	NAD	O4B-C4B-C5B-O5B

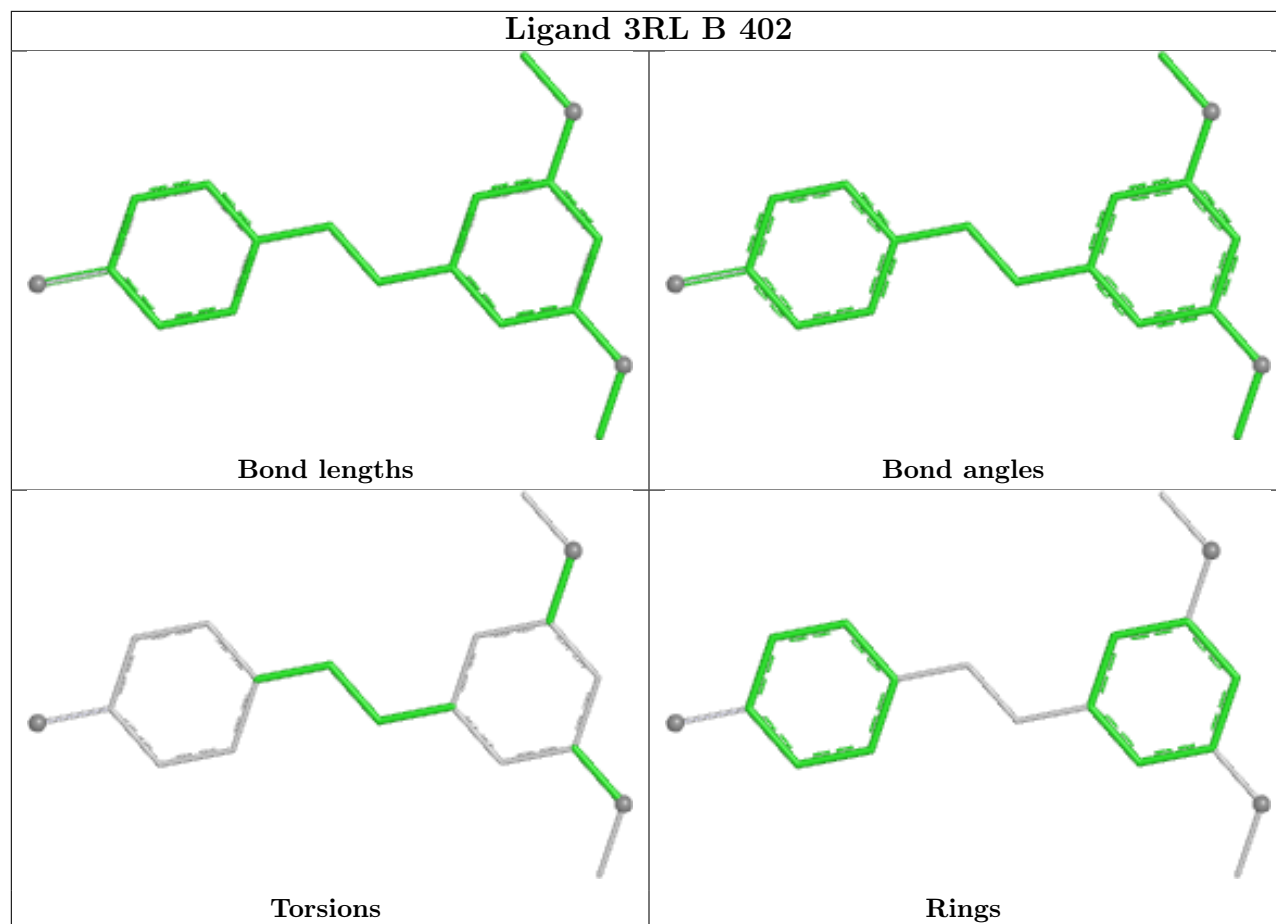
There are no ring outliers.

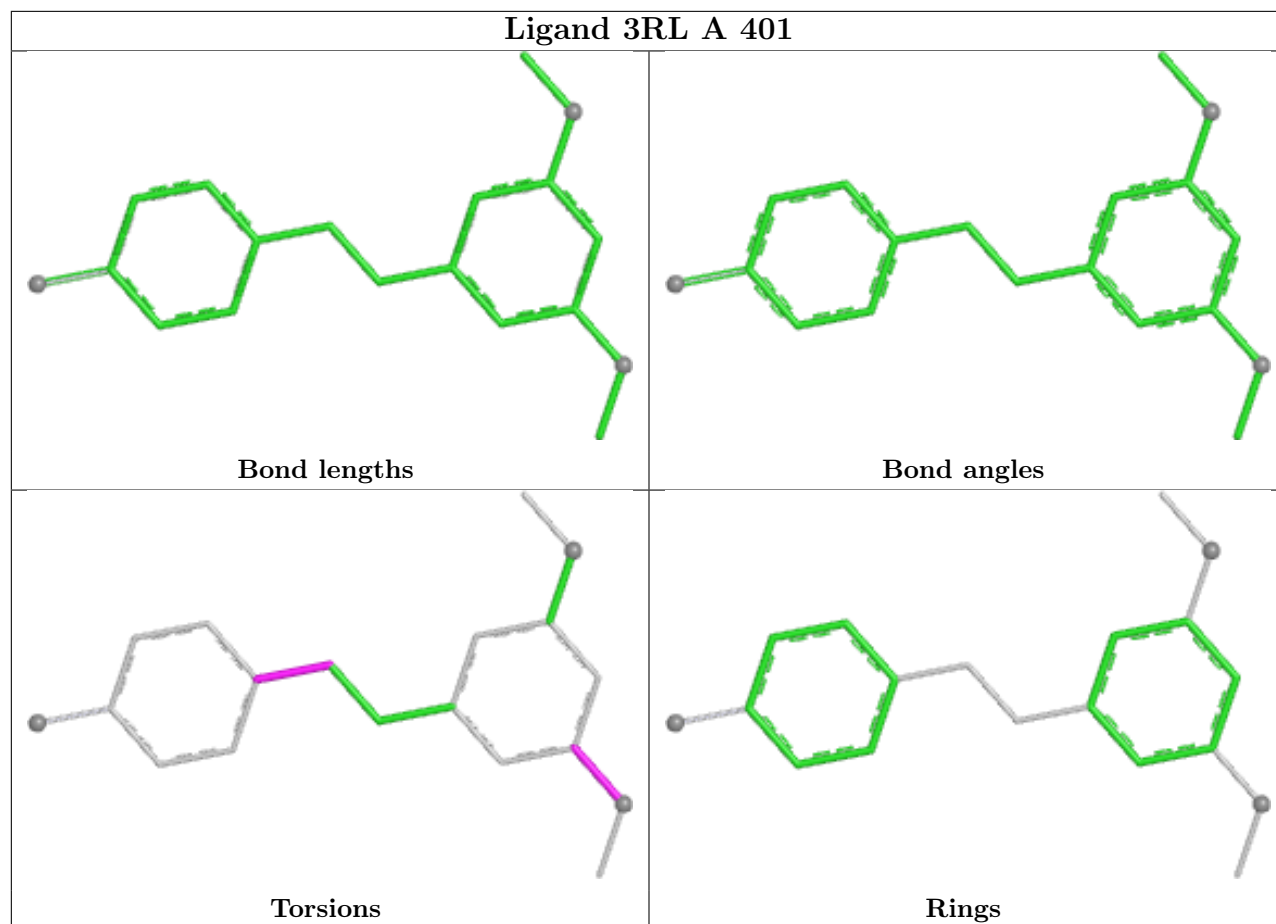
9 monomers are involved in 28 short contacts:

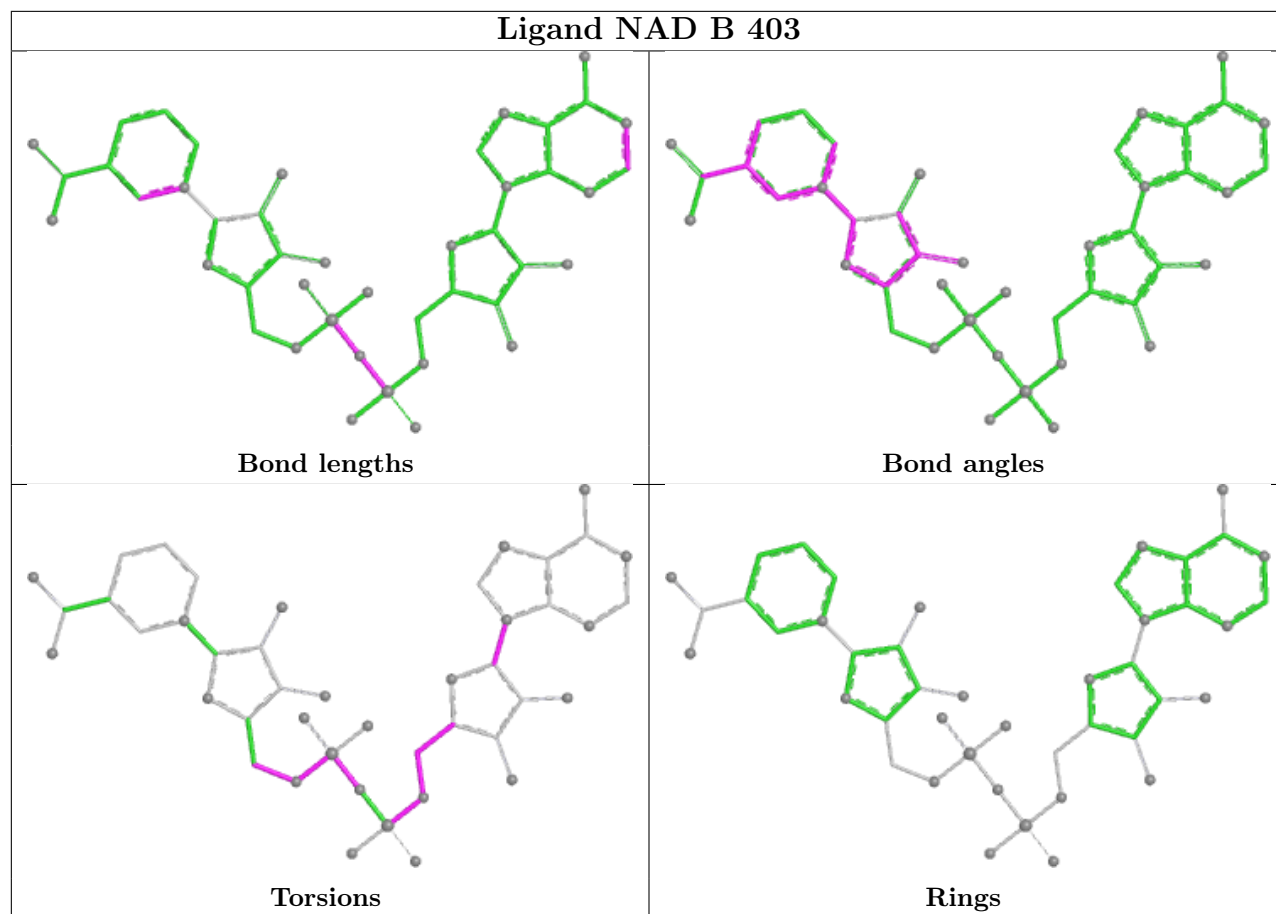
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	3RL	5	0
5	A	405	PG4	3	0
6	A	406	PEG	3	0
4	B	409	GOL	2	0
4	B	407	GOL	6	0
3	B	403	NAD	8	0
4	B	404	GOL	1	0
3	A	402	NAD	1	0
7	A	407	EDO	2	0

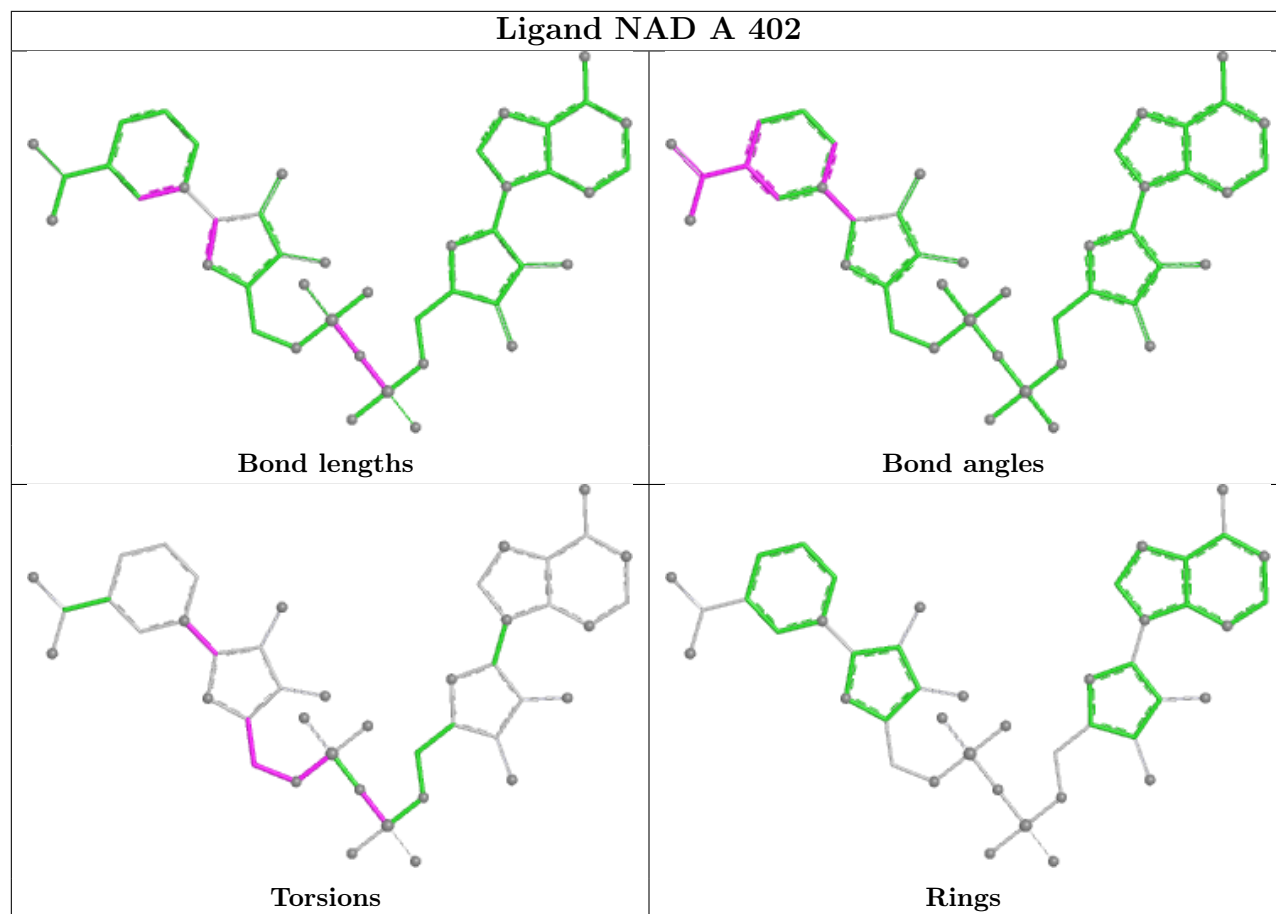
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 3RL B 402









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	363/376 (96%)	0.58	38 (10%) 11 8	16, 41, 94, 155	6 (1%)
1	B	363/376 (96%)	0.32	23 (6%) 26 22	16, 37, 90, 143	6 (1%)
All	All	726/752 (96%)	0.45	61 (8%) 17 14	16, 39, 94, 155	12 (1%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	VAL	6.6
1	A	112	THR	6.4
1	A	302	VAL	5.7
1	A	132	GLY	5.7
1	A	301	HIS	5.3
1	A	106	THR	5.1
1	A	304	GLY	4.8
1	A	16	ALA	4.6
1	B	113	THR	4.5
1	B	104	VAL	4.4
1	A	104	VAL	4.4
1	B	109	ALA	4.2
1	A	255	VAL	4.1
1	B	115	CYS	4.0
1	A	272	GLY	3.9
1	B	133	VAL	3.9
1	A	110	THR	3.8
1	A	113	THR	3.8
1	A	18	ASN	3.7
1	B	111	THR	3.7
1	B	112	THR	3.6
1	A	254	PRO	3.6
1	A	109	ALA	3.4
1	B	110	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	16	ALA	3.3
1	A	15	SER	3.3
1	A	108	ASP	3.2
1	B	135	ASP	3.1
1	A	131	ASN	3.1
1	B	18	ASN	3.1
1	A	250	ALA	3.1
1	A	114	CYS	3.0
1	A	107	ASP	3.0
1	A	316[A]	GLU	2.9
1	B	105	GLY	2.9
1	A	135	ASP	2.8
1	B	252	ALA	2.7
1	A	315[A]	ASP	2.6
1	A	246	PRO	2.6
1	A	224	ASN	2.6
1	A	245	LEU	2.6
1	B	106	THR	2.6
1	A	271	ARG	2.5
1	A	252	ALA	2.5
1	A	62	GLU	2.5
1	B	114	CYS	2.5
1	A	103	VAL	2.5
1	A	262	GLY	2.5
1	B	249	ILE	2.5
1	A	377	LYS	2.5
1	A	115	CYS	2.4
1	A	267	ASP	2.4
1	B	103	VAL	2.4
1	B	132	GLY	2.3
1	B	19	GLU	2.2
1	A	241	ILE	2.1
1	B	303	ARG	2.1
1	B	302	VAL	2.1
1	B	250	ALA	2.1
1	A	249	ILE	2.1
1	B	254	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

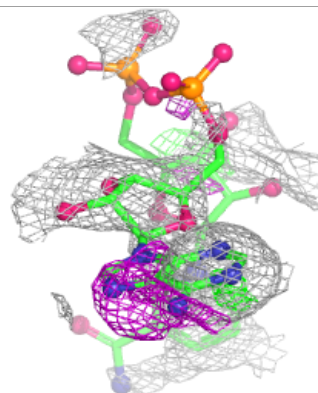
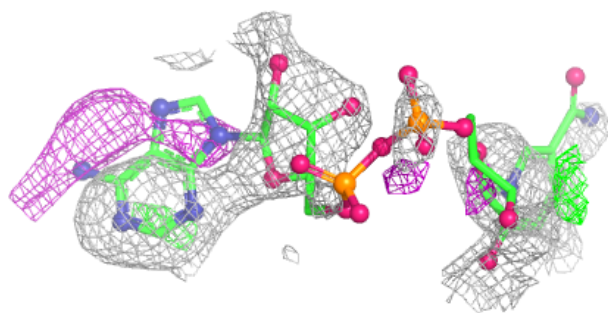
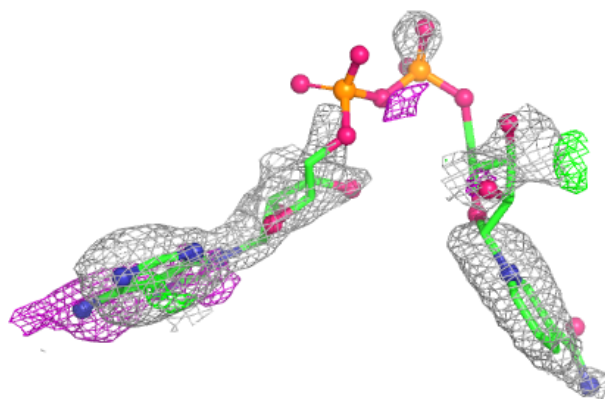
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAD	B	403	44/44	0.68	0.24	38,111,153,176	0
4	GOL	B	408	6/6	0.74	0.20	78,79,94,97	0
7	EDO	B	406	4/4	0.75	0.19	55,61,67,69	0
3	NAD	A	402	44/44	0.77	0.17	50,73,126,132	0
7	EDO	A	407	4/4	0.78	0.19	54,62,64,70	0
4	GOL	A	403	6/6	0.78	0.18	46,50,66,73	0
7	EDO	A	408	4/4	0.79	0.28	48,58,63,63	0
6	PEG	A	406	7/7	0.81	0.19	60,70,80,81	0
4	GOL	B	407	6/6	0.82	0.21	53,57,66,67	0
4	GOL	B	410	6/6	0.83	0.14	64,71,76,79	0
5	PG4	A	405	13/13	0.83	0.20	40,71,117,126	0
7	EDO	B	411	4/4	0.83	0.25	66,66,67,70	0
4	GOL	B	401	6/6	0.84	0.17	49,59,68,70	0
7	EDO	B	405	4/4	0.84	0.16	68,69,80,93	0
4	GOL	B	409	6/6	0.85	0.14	48,65,68,71	0
2	3RL	A	401	19/19	0.87	0.12	38,46,59,63	0
4	GOL	A	404	6/6	0.88	0.12	40,48,49,56	0
2	3RL	B	402	19/19	0.89	0.11	39,45,54,57	0
4	GOL	B	404	6/6	0.91	0.18	53,54,60,68	0

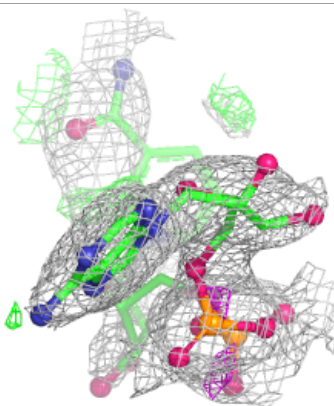
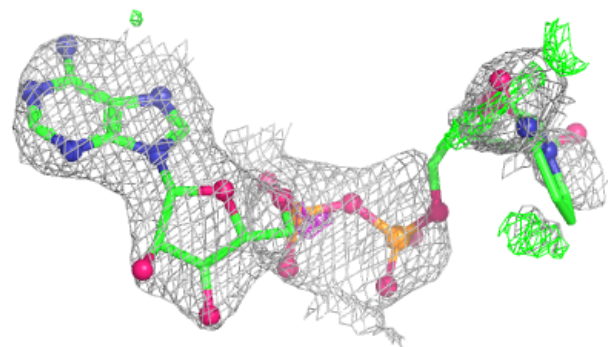
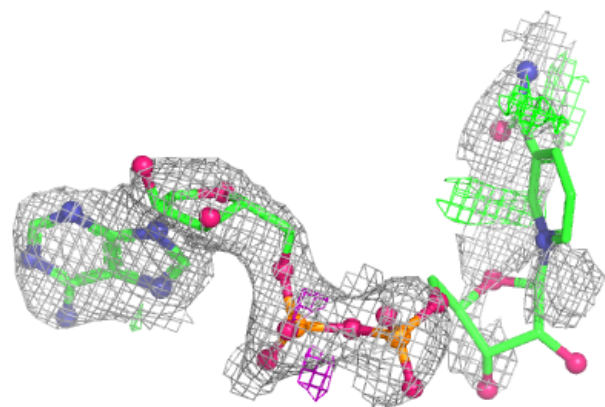
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD 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)

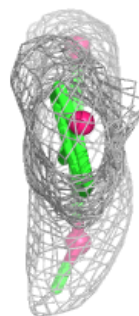
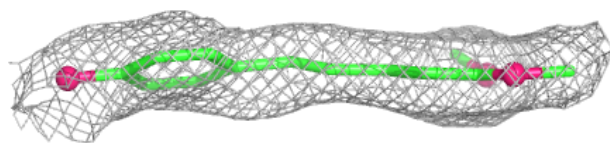
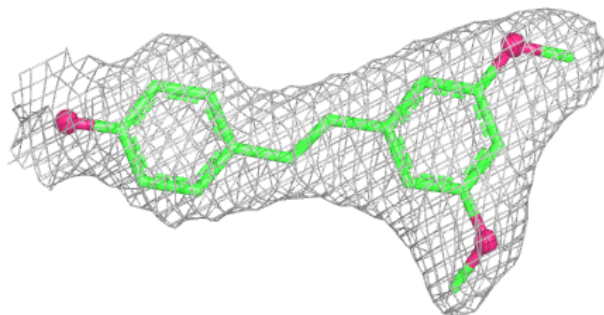
**Electron density around NAD A 402:**

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

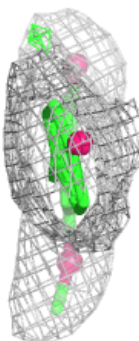
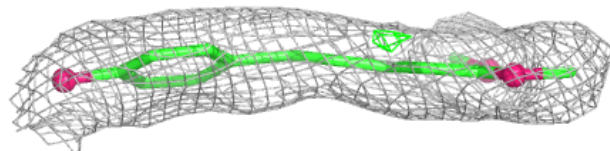
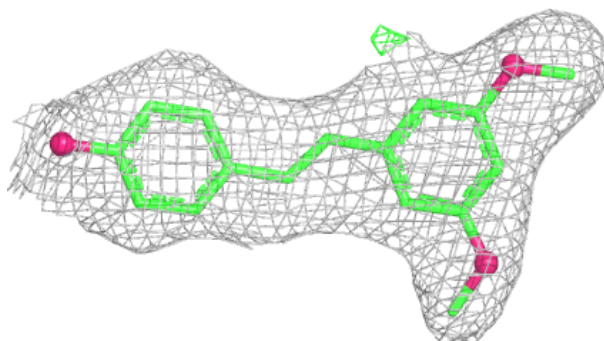


Electron density around 3RL A 401:

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

**Electron density around 3RL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.