



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:59 PM UTC

PDB ID : 2X1H / pdb_00002x1h
Title : Crystal structure of the human MGC45594 gene product in complex with raloxifene
Authors : Shafqat, N.; Yue, W.W.; Pike, A.C.W.; Niesen, F.; Ugochukwu, E.; Krojer, T.; Chaikuad, A.; Smee, C.; Arrowsmith, C.; Weigelt, J.; Edwards, A.; Bountra, C.; Oppermann, U.
Deposited on : 2009-12-24
Resolution : 1.75 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](#) ①) 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

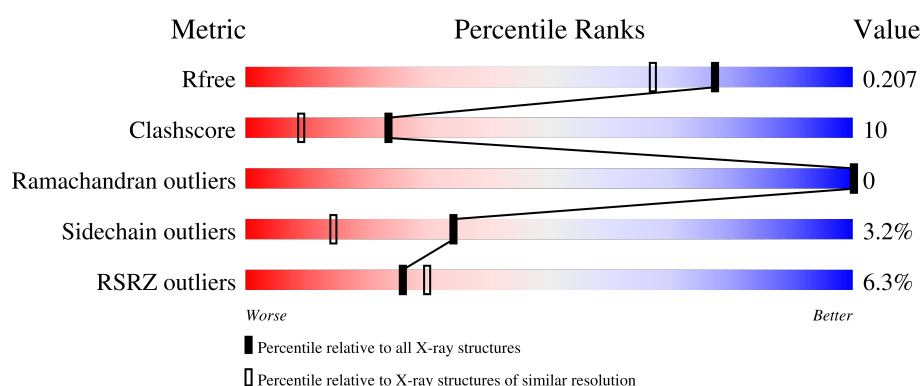
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	362	
1	B	362	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5824 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 ZINC-BINDING ALCOHOL DEHYDROGENASE DOMAIN-CONTAINING PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	6	0
			2524	1620	405	485	14			
1	B	339	Total	C	N	O	S	0	3	0
			2501	1602	405	480	14			

There are 46 discrepancies between the modelled and reference sequences:

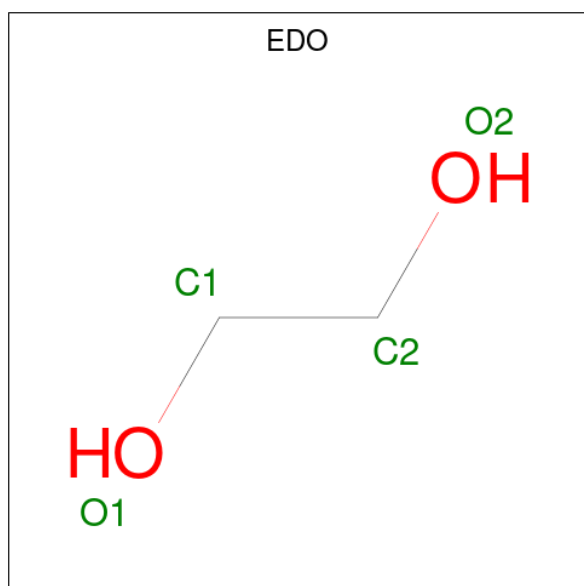
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q8N4Q0
A	2	HIS	-	expression tag	UNP Q8N4Q0
A	3	HIS	-	expression tag	UNP Q8N4Q0
A	4	HIS	-	expression tag	UNP Q8N4Q0
A	5	HIS	-	expression tag	UNP Q8N4Q0
A	6	HIS	-	expression tag	UNP Q8N4Q0
A	7	HIS	-	expression tag	UNP Q8N4Q0
A	8	SER	-	expression tag	UNP Q8N4Q0
A	9	SER	-	expression tag	UNP Q8N4Q0
A	10	GLY	-	expression tag	UNP Q8N4Q0
A	11	VAL	-	expression tag	UNP Q8N4Q0
A	12	ASP	-	expression tag	UNP Q8N4Q0
A	13	LEU	-	expression tag	UNP Q8N4Q0
A	14	GLY	-	expression tag	UNP Q8N4Q0
A	15	THR	-	expression tag	UNP Q8N4Q0
A	16	GLU	-	expression tag	UNP Q8N4Q0
A	17	ASN	-	expression tag	UNP Q8N4Q0
A	18	LEU	-	expression tag	UNP Q8N4Q0
A	19	TYR	-	expression tag	UNP Q8N4Q0
A	20	PHE	-	expression tag	UNP Q8N4Q0
A	21	GLN	-	expression tag	UNP Q8N4Q0
A	22	SER	-	expression tag	UNP Q8N4Q0
A	23	MET	-	expression tag	UNP Q8N4Q0
B	1	MET	-	expression tag	UNP Q8N4Q0

Continued on next page...

Continued from previous page...

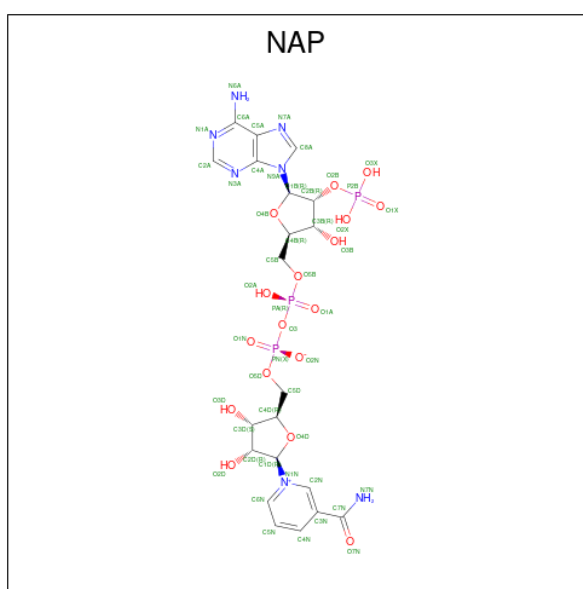
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	HIS	-	expression tag	UNP Q8N4Q0
B	3	HIS	-	expression tag	UNP Q8N4Q0
B	4	HIS	-	expression tag	UNP Q8N4Q0
B	5	HIS	-	expression tag	UNP Q8N4Q0
B	6	HIS	-	expression tag	UNP Q8N4Q0
B	7	HIS	-	expression tag	UNP Q8N4Q0
B	8	SER	-	expression tag	UNP Q8N4Q0
B	9	SER	-	expression tag	UNP Q8N4Q0
B	10	GLY	-	expression tag	UNP Q8N4Q0
B	11	VAL	-	expression tag	UNP Q8N4Q0
B	12	ASP	-	expression tag	UNP Q8N4Q0
B	13	LEU	-	expression tag	UNP Q8N4Q0
B	14	GLY	-	expression tag	UNP Q8N4Q0
B	15	THR	-	expression tag	UNP Q8N4Q0
B	16	GLU	-	expression tag	UNP Q8N4Q0
B	17	ASN	-	expression tag	UNP Q8N4Q0
B	18	LEU	-	expression tag	UNP Q8N4Q0
B	19	TYR	-	expression tag	UNP Q8N4Q0
B	20	PHE	-	expression tag	UNP Q8N4Q0
B	21	GLN	-	expression tag	UNP Q8N4Q0
B	22	SER	-	expression tag	UNP Q8N4Q0
B	23	MET	-	expression tag	UNP Q8N4Q0

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



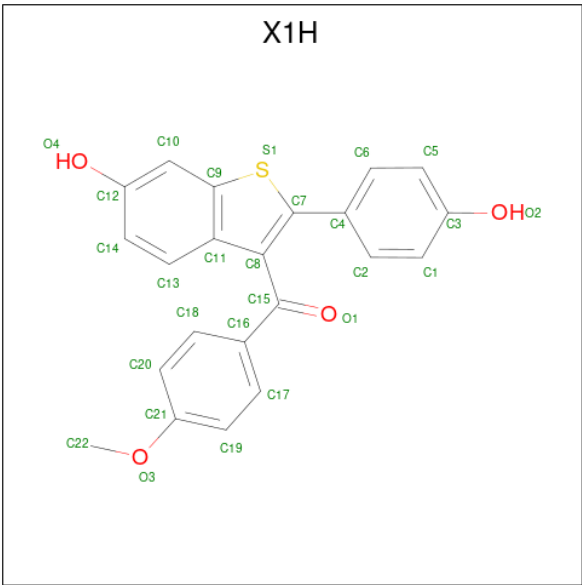
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is [6-HYDROXY-2-(4-HYDROXYPHENYL)-1-BENZOTHIOPHEN-3-YL](4-METHOXYPHENYL)METHANONE (CCD ID: X1H) (formula: C₂₂H₁₆O₄S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			26	21	4	1		
4	A	1	Total	C	O	S	0	0
			27	22	4	1		
4	B	1	Total	C	O	S	0	0
			26	21	4	1		
4	B	1	Total	C	O	S	0	0
			26	21	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	318	Total	O	0	0
			318	318		
5	B	264	Total	O	0	0
			264	264		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.65Å 52.04Å 75.44Å 94.32° 91.44° 102.24°	Depositor
Resolution (Å)	40.50 – 1.75 40.50 – 1.75	Depositor EDS
% Data completeness (in resolution range)	92.7 (40.50-1.75) 92.7 (40.50-1.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.75Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.208 , 0.243 0.206 , 0.207	Depositor DCC
R_{free} test set	1831 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5824	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, X1H, NAP

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	0.43	0/2600	0.78	1/3534 (0.0%)
1	B	0.42	0/2564	0.78	2/3485 (0.1%)
All	All	0.43	0/5164	0.78	3/7019 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	MET	CG-SD-CE	-6.42	86.78	100.90
1	B	181	MET	CG-SD-CE	-6.05	87.58	100.90
1	B	312	GLU	CA-CB-CG	-5.57	102.95	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2524	0	2536	57	0
1	B	2501	0	2500	42	0
2	A	12	0	18	5	0
2	B	4	0	6	1	0
3	A	48	0	25	5	0
3	B	48	0	25	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	53	0	29	2	0
4	B	52	0	26	1	0
5	A	318	0	0	29	0
5	B	264	0	0	15	0
All	All	5824	0	5165	106	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 10.

All (106) 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:357:VAL:HA	5:A:3040:HOH:O	1.42	1.17
1:B:181:MET:HE1	1:B:209:CYS:CB	1.82	1.08
1:A:181:MET:HE1	1:A:209:CYS:CB	1.85	1.06
1:A:255:GLY:HA2	5:A:3217:HOH:O	1.58	1.00
1:A:64:GLY:HA2	5:A:3040:HOH:O	1.66	0.95
1:A:181:MET:HE1	1:A:209:CYS:CA	1.98	0.93
1:B:304:GLN:HG3	5:B:3220:HOH:O	1.70	0.91
1:B:181:MET:HE1	1:B:209:CYS:HB2	1.50	0.90
1:A:181:MET:HE1	1:A:209:CYS:HB2	1.54	0.88
1:B:181:MET:HE1	1:B:209:CYS:CA	2.04	0.88
1:A:135:PRO:HG3	2:A:1363:EDO:H21	1.57	0.87
1:B:181:MET:CE	1:B:209:CYS:HB2	2.05	0.85
1:A:181:MET:CE	1:A:209:CYS:HB2	2.07	0.84
1:B:105:ARG:HD3	5:B:3069:HOH:O	1.79	0.83
1:B:38:GLU:HB2	5:B:3009:HOH:O	1.80	0.81
1:A:257:LEU:CD1	5:A:3210:HOH:O	2.29	0.81
1:A:276:LYS:HE3	5:A:3233:HOH:O	1.82	0.79
1:A:238:SER:HB3	3:A:1372:NAP:H4D	1.64	0.78
1:B:241:GLY:HA2	5:B:3199:HOH:O	1.83	0.77
1:B:260:ILE:O	3:B:1372:NAP:H2N	1.85	0.75
2:A:1362:EDO:H12	5:A:3217:HOH:O	1.87	0.75
1:B:238:SER:HB3	3:B:1372:NAP:H4D	1.69	0.74
1:A:248:VAL:N	5:A:3210:HOH:O	2.20	0.74
1:A:247:ALA:HB3	5:A:3210:HOH:O	1.90	0.72
3:A:1372:NAP:H8A	3:A:1372:NAP:H3B	1.71	0.72
2:A:1362:EDO:C1	5:A:3217:HOH:O	2.38	0.72
1:A:257:LEU:HD12	5:A:3210:HOH:O	1.90	0.72
1:A:112[B]:VAL:HG11	1:A:131:ALA:HB1	1.73	0.71
1:A:63:VAL:O	5:A:3040:HOH:O	2.09	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:MET:HE1	1:A:209:CYS:HA	1.70	0.70
1:A:181:MET:CE	1:A:209:CYS:CB	2.66	0.69
1:A:133:PRO:HB3	5:A:3091:HOH:O	1.91	0.69
1:A:315:VAL:HB	5:A:3269:HOH:O	1.94	0.68
1:A:76:ARG:N	5:A:3048:HOH:O	2.26	0.68
1:A:312:GLU:HA	5:A:3269:HOH:O	1.94	0.67
1:B:44:ARG:HG2	1:B:44:ARG:HH11	1.59	0.67
1:A:345:ASN:HB2	2:A:1364:EDO:H21	1.75	0.67
1:B:181:MET:CE	1:B:209:CYS:CB	2.65	0.67
1:B:181:MET:HE1	1:B:209:CYS:HA	1.78	0.66
1:A:257:LEU:HD11	5:A:3210:HOH:O	1.91	0.65
1:A:71:ASN:O	5:A:3048:HOH:O	2.14	0.65
1:A:256:ARG:HB3	5:A:3242:HOH:O	1.97	0.65
1:A:44:ARG:HH11	1:A:44:ARG:CG	2.10	0.63
1:A:103:SER:O	5:A:3082:HOH:O	2.16	0.63
1:B:44:ARG:HH11	1:B:44:ARG:CG	2.10	0.63
1:A:94[A]:GLU:HG2	5:A:3077:HOH:O	1.99	0.62
1:A:260:ILE:O	3:A:1372:NAP:H2N	2.02	0.60
1:B:35:ASN:HB3	5:B:3009:HOH:O	2.02	0.59
1:B:144:LEU:HB2	1:B:307:MET:HE1	1.84	0.57
1:A:98:LEU:HD11	1:A:103:SER:HA	1.86	0.57
1:B:241:GLY:CA	5:B:3199:HOH:O	2.49	0.57
1:A:188:LYS:HE3	5:A:3166:HOH:O	2.05	0.57
1:A:186:LYS:HD3	4:A:2002:X1H:C10	2.34	0.56
1:B:98:LEU:HD11	1:B:103:SER:HA	1.88	0.56
1:A:112[B]:VAL:CG1	1:A:131:ALA:HB1	2.36	0.55
1:A:144:LEU:HB2	1:A:307:MET:HE1	1.87	0.55
2:B:1362:EDO:H11	3:B:1372:NAP:H4N	1.87	0.55
1:B:181:MET:HE1	1:B:209:CYS:SG	2.48	0.53
1:A:44:ARG:HH11	1:A:44:ARG:HG2	1.74	0.52
1:A:345:ASN:CB	2:A:1364:EDO:H21	2.41	0.51
1:B:35:ASN:HB2	5:B:3011:HOH:O	2.09	0.51
1:B:345[B]:ASN:ND2	5:B:3249:HOH:O	2.37	0.51
1:A:72:TYR:HA	5:A:3048:HOH:O	2.10	0.51
1:A:280:LEU:HB3	1:A:281:PRO:HD3	1.93	0.51
1:A:347:MET:HB2	1:A:356:ILE:HD12	1.93	0.51
1:A:29:VAL:O	1:A:84:PRO:HA	2.10	0.50
1:B:29:VAL:O	1:B:84:PRO:HA	2.11	0.50
1:B:113:ALA:HB1	1:B:145:LEU:HD11	1.94	0.50
1:A:138:LYS:NZ	5:A:3127:HOH:O	2.45	0.50
1:B:347:MET:HB2	1:B:356:ILE:HD12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:CZ	5:B:3086:HOH:O	2.60	0.49
1:A:276:LYS:NZ	5:A:3234:HOH:O	2.46	0.49
1:A:113:ALA:HB1	1:A:145:LEU:HD11	1.95	0.49
1:A:325:LEU:HD23	1:A:357:VAL:O	2.12	0.49
1:B:187:ALA:HA	4:B:2002:X1H:O1	2.13	0.48
1:A:37:ARG:HA	1:A:37:ARG:HD3	1.60	0.48
1:B:325:LEU:HD23	1:B:357:VAL:O	2.14	0.48
1:B:274:PRO:N	5:B:3199:HOH:O	2.48	0.47
1:A:181:MET:HE1	1:A:209:CYS:SG	2.54	0.47
1:B:37:ARG:HD3	1:B:37:ARG:HA	1.60	0.47
1:A:258[B]:ILE:HD11	5:A:3147:HOH:O	2.15	0.47
1:B:256:ARG:NE	5:B:3186:HOH:O	2.48	0.46
1:B:166:LYS:NZ	5:B:3123:HOH:O	2.45	0.46
1:A:257:LEU:C	1:A:257:LEU:HD23	2.41	0.46
1:B:23:MET:N	5:B:3004:HOH:O	2.49	0.45
1:A:186:LYS:NZ	1:A:318[B]:ASP:OD1	2.48	0.45
1:A:247:ALA:C	5:A:3210:HOH:O	2.59	0.45
1:B:257:LEU:HD23	1:B:257:LEU:C	2.42	0.45
1:A:247:ALA:CB	5:A:3210:HOH:O	2.57	0.45
1:B:44:ARG:HG2	1:B:44:ARG:NH1	2.31	0.45
1:A:44:ARG:CG	1:A:44:ARG:NH1	2.77	0.44
3:A:1372:NAP:H8A	3:A:1372:NAP:C3B	2.44	0.44
1:A:330:PRO:HD2	5:A:3311:HOH:O	2.18	0.43
1:B:199:GLU:N	1:B:199:GLU:OE1	2.50	0.43
1:B:280:LEU:HB3	1:B:281:PRO:HD3	2.01	0.43
1:B:285:LEU:C	1:B:285:LEU:HD23	2.44	0.43
1:B:182:GLN:O	1:B:186:LYS:HG3	2.18	0.43
1:B:349:MET:HE2	1:B:349:MET:HA	2.00	0.43
1:B:334:PHE:HB3	1:B:358:VAL:HG22	2.01	0.42
1:A:349:MET:HA	1:A:349:MET:HE2	2.01	0.42
1:B:359:GLU:CD	5:B:3255:HOH:O	2.63	0.42
4:A:2001:X1H:C4	5:A:3315:HOH:O	2.68	0.41
3:A:1372:NAP:C3B	3:A:1372:NAP:C8A	2.98	0.41
1:B:274:PRO:HD2	5:B:3199:HOH:O	2.21	0.40
1:A:33:SER:HA	1:A:34:PRO:HD3	1.87	0.40
1:A:285:LEU:HD23	1:A:285:LEU:C	2.47	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	344/362 (95%)	338 (98%)	6 (2%)	0	100	100
1	B	340/362 (94%)	335 (98%)	5 (2%)	0	100	100
All	All	684/724 (94%)	673 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	273/296 (92%)	263 (96%)	10 (4%)	30	11
1	B	268/296 (90%)	259 (97%)	9 (3%)	32	13
All	All	541/592 (91%)	522 (96%)	19 (4%)	34	12

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	37	ARG
1	A	44	ARG
1	A	59	ARG
1	A	68[A]	SER
1	A	68[B]	SER
1	A	181	MET
1	A	237	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	311	LEU
1	A	349	MET
1	B	37	ARG
1	B	44	ARG
1	B	59	ARG
1	B	68[A]	SER
1	B	68[B]	SER
1	B	181	MET
1	B	237	GLU
1	B	311	LEU
1	B	349	MET

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

Mol	Chain	Res	Type
1	A	60	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	X1H	A	2001	-	29,29,30	5.22	12 (41%)	41,42,43	4.05	9 (21%)
2	EDO	B	1362	-	3,3,3	0.43	0	2,2,2	0.47	0
4	X1H	B	2002	-	29,29,30	5.29	13 (44%)	41,42,43	3.71	10 (24%)
3	NAP	A	1372	-	50,52,52	1.90	13 (26%)	71,80,80	1.60	14 (19%)
2	EDO	A	1363	-	3,3,3	0.43	0	2,2,2	0.39	0
3	NAP	B	1372	-	50,52,52	1.92	15 (30%)	71,80,80	1.49	13 (18%)
2	EDO	A	1362	-	3,3,3	0.44	0	2,2,2	0.29	0
2	EDO	A	1364	-	3,3,3	0.42	0	2,2,2	0.40	0
4	X1H	B	2001	-	29,29,30	5.14	14 (48%)	41,42,43	3.99	11 (26%)
4	X1H	A	2002	-	30,30,30	5.10	11 (36%)	42,43,43	3.75	13 (30%)

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	X1H	A	2001	-	-	2/12/12/14	0/4/4/4
2	EDO	B	1362	-	-	0/1/1/1	-
4	X1H	B	2002	-	-	0/12/12/14	0/4/4/4
3	NAP	A	1372	-	-	5/35/67/67	0/5/5/5
2	EDO	A	1363	-	-	0/1/1/1	-
3	NAP	B	1372	-	-	4/35/67/67	0/5/5/5
2	EDO	A	1362	-	-	1/1/1/1	-
2	EDO	A	1364	-	-	0/1/1/1	-
4	X1H	B	2001	-	-	0/12/12/14	0/4/4/4
4	X1H	A	2002	-	-	2/14/14/14	0/4/4/4

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2002	X1H	C8-C7	18.21	1.61	1.37
4	A	2001	X1H	C8-C7	18.19	1.61	1.37
4	A	2002	X1H	C8-C7	17.58	1.60	1.37
4	B	2001	X1H	C8-C7	17.52	1.60	1.37
4	B	2002	X1H	C7-S1	-14.91	1.56	1.74
4	A	2002	X1H	C7-S1	-14.78	1.56	1.74
4	B	2001	X1H	C7-S1	-14.26	1.57	1.74
4	A	2001	X1H	C7-S1	-14.11	1.57	1.74
4	A	2001	X1H	C11-C9	8.72	1.54	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2002	X1H	C11-C9	8.70	1.54	1.41
4	A	2002	X1H	C11-C9	8.36	1.53	1.41
4	B	2001	X1H	C11-C9	8.24	1.53	1.41
4	A	2001	X1H	C11-C8	6.78	1.62	1.46
4	A	2002	X1H	C6-C4	6.73	1.49	1.39
4	B	2002	X1H	C11-C8	6.69	1.61	1.46
4	A	2001	X1H	C6-C4	6.67	1.49	1.39
4	B	2001	X1H	C6-C4	6.67	1.49	1.39
4	B	2001	X1H	C11-C8	6.57	1.61	1.46
4	A	2002	X1H	C11-C8	6.33	1.61	1.46
4	B	2002	X1H	C6-C4	6.17	1.48	1.39
3	B	1372	NAP	O4D-C1D	-5.83	1.33	1.40
4	B	2001	X1H	C19-C21	5.33	1.49	1.39
4	B	2002	X1H	C19-C21	5.32	1.48	1.39
4	A	2001	X1H	C19-C21	5.23	1.48	1.39
4	A	2002	X1H	C19-C21	5.14	1.48	1.38
3	A	1372	NAP	C5A-N7A	-4.73	1.30	1.39
3	A	1372	NAP	C3N-C7N	4.33	1.57	1.50
3	B	1372	NAP	C5A-N7A	-4.26	1.31	1.39
3	A	1372	NAP	PA-O2A	-4.00	1.36	1.55
4	B	2002	X1H	C14-C12	3.74	1.46	1.39
3	B	1372	NAP	PA-O1A	-3.67	1.38	1.50
3	A	1372	NAP	C4A-N9A	-3.65	1.30	1.37
4	A	2001	X1H	C14-C12	3.36	1.45	1.39
4	B	2001	X1H	C14-C12	3.34	1.45	1.39
3	A	1372	NAP	PN-O2N	-3.33	1.39	1.55
3	A	1372	NAP	P2B-O1X	-3.33	1.40	1.50
4	A	2002	X1H	C14-C12	3.23	1.45	1.39
3	A	1372	NAP	PN-O3	3.22	1.63	1.59
3	B	1372	NAP	PA-O2A	-3.18	1.40	1.55
3	B	1372	NAP	C4A-N9A	-3.16	1.31	1.37
3	B	1372	NAP	C8A-N9A	-3.15	1.32	1.37
4	A	2002	X1H	C10-C12	3.14	1.43	1.39
3	A	1372	NAP	PA-O1A	-3.01	1.40	1.50
4	B	2001	X1H	C13-C11	-2.96	1.35	1.39
3	B	1372	NAP	PN-O2N	-2.95	1.41	1.55
3	A	1372	NAP	C8A-N9A	-2.94	1.32	1.37
4	B	2001	X1H	C18-C16	2.91	1.43	1.39
4	A	2002	X1H	C13-C11	-2.90	1.35	1.39
3	B	1372	NAP	P2B-O1X	-2.88	1.41	1.50
4	B	2001	X1H	C1-C3	2.84	1.44	1.39
4	A	2001	X1H	C10-C12	2.80	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2002	X1H	C18-C16	2.76	1.43	1.39
4	A	2001	X1H	C18-C16	2.76	1.43	1.39
4	B	2002	X1H	C10-C12	2.75	1.43	1.39
4	A	2002	X1H	C18-C16	2.72	1.43	1.39
3	B	1372	NAP	PA-O5B	-2.70	1.48	1.59
4	B	2002	X1H	C13-C11	-2.66	1.35	1.39
3	B	1372	NAP	C2N-N1N	2.65	1.37	1.35
4	A	2001	X1H	C13-C11	-2.63	1.36	1.39
4	A	2001	X1H	C1-C3	2.53	1.43	1.39
4	A	2002	X1H	C1-C3	2.46	1.43	1.39
4	B	2002	X1H	C1-C3	2.37	1.43	1.39
4	B	2001	X1H	C10-C12	2.29	1.42	1.39
3	B	1372	NAP	O5D-C5D	-2.27	1.36	1.44
3	A	1372	NAP	C6N-N1N	2.27	1.40	1.35
4	B	2001	X1H	C9-S1	-2.26	1.69	1.74
3	A	1372	NAP	P2B-O2B	2.23	1.63	1.59
4	B	2001	X1H	C10-C9	-2.21	1.35	1.39
4	B	2002	X1H	C14-C13	2.21	1.42	1.38
3	B	1372	NAP	O4B-C4B	-2.20	1.40	1.45
3	B	1372	NAP	O5B-C5B	-2.20	1.36	1.44
3	A	1372	NAP	O4D-C1D	-2.19	1.38	1.40
3	A	1372	NAP	C2N-N1N	2.16	1.37	1.35
4	A	2001	X1H	C14-C13	2.14	1.42	1.38
3	B	1372	NAP	C3N-C7N	2.12	1.53	1.50
4	B	2002	X1H	C9-S1	-2.09	1.70	1.74
3	B	1372	NAP	O4D-C4D	-2.06	1.40	1.45
4	B	2001	X1H	C18-C20	2.01	1.42	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	X1H	C9-S1-C7	21.79	107.30	90.58
4	B	2001	X1H	C9-S1-C7	21.06	106.73	90.58
4	B	2002	X1H	C9-S1-C7	20.69	106.45	90.58
4	A	2002	X1H	C9-S1-C7	20.08	105.98	90.58
4	B	2001	X1H	C4-C7-S1	8.40	130.05	117.69
4	A	2001	X1H	C4-C7-S1	7.82	129.20	117.69
4	A	2002	X1H	C11-C8-C7	-5.59	108.48	112.51
4	A	2002	X1H	C4-C7-S1	5.44	125.69	117.69
4	B	2002	X1H	C11-C8-C7	-5.37	108.64	112.51
4	B	2001	X1H	C4-C7-C8	-5.32	122.05	130.17
3	A	1372	NAP	C5A-C4A-N3A	-5.28	119.44	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	X1H	C8-C7-S1	-5.03	107.59	112.04
4	B	2001	X1H	C8-C7-S1	-4.82	107.78	112.04
4	B	2002	X1H	C4-C7-S1	4.81	124.77	117.69
4	A	2001	X1H	C11-C8-C7	-4.80	109.05	112.51
4	A	2001	X1H	C4-C7-C8	-4.73	122.95	130.17
3	A	1372	NAP	N3A-C2A-N1A	-4.66	121.53	128.58
3	B	1372	NAP	C5A-C4A-N3A	-4.63	120.34	126.72
4	B	2001	X1H	C11-C8-C7	-4.50	109.27	112.51
4	A	2002	X1H	C10-C9-C11	-4.28	118.03	121.74
4	A	2001	X1H	C11-C9-S1	-4.14	107.37	112.24
4	B	2002	X1H	C8-C7-S1	-3.97	108.53	112.04
4	A	2002	X1H	C11-C9-S1	-3.95	107.59	112.24
3	B	1372	NAP	N3A-C2A-N1A	-3.73	122.93	128.58
3	A	1372	NAP	C2A-N3A-C4A	3.72	120.93	111.83
3	B	1372	NAP	C4A-C5A-N7A	-3.70	106.35	110.58
4	A	2001	X1H	C10-C9-C11	-3.61	118.61	121.74
4	B	2001	X1H	C11-C9-S1	-3.60	108.00	112.24
4	A	2002	X1H	C8-C7-S1	-3.50	108.95	112.04
4	B	2002	X1H	C11-C9-S1	-3.48	108.15	112.24
4	A	2002	X1H	C4-C7-C8	-3.44	124.92	130.17
4	B	2002	X1H	C10-C9-C11	-3.43	118.76	121.74
4	A	2002	X1H	C10-C9-S1	3.33	134.38	126.07
3	A	1372	NAP	C4A-C5A-N7A	-3.30	106.81	110.58
4	A	2001	X1H	C10-C9-S1	3.18	134.01	126.07
4	B	2001	X1H	C10-C9-C11	-3.15	119.01	121.74
4	A	2002	X1H	C6-C4-C7	-3.15	115.84	120.84
3	B	1372	NAP	C2A-N3A-C4A	3.11	119.43	111.83
4	B	2001	X1H	C9-C11-C8	-2.99	108.22	111.47
4	B	2002	X1H	C9-C11-C8	-2.98	108.24	111.47
3	A	1372	NAP	N3A-C4A-N9A	2.96	132.20	127.17
3	A	1372	NAP	C5A-N7A-C8A	2.82	107.88	103.45
4	B	2002	X1H	C10-C9-S1	2.81	133.09	126.07
4	A	2002	X1H	C1-C2-C4	-2.80	117.81	120.80
3	B	1372	NAP	C5A-N7A-C8A	2.77	107.80	103.45
4	B	2001	X1H	C10-C9-S1	2.77	132.97	126.07
3	A	1372	NAP	N9A-C8A-N7A	-2.67	110.15	113.94
3	B	1372	NAP	C5A-C4A-N9A	2.61	108.66	105.81
3	B	1372	NAP	C4D-O4D-C1D	-2.60	107.54	109.92
3	A	1372	NAP	O7N-C7N-C3N	2.58	122.75	119.60
4	A	2001	X1H	C9-C11-C8	-2.56	108.69	111.47
3	A	1372	NAP	C5D-C4D-C3D	-2.55	106.03	115.21
3	A	1372	NAP	C4D-O4D-C1D	-2.43	107.70	109.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2002	X1H	C6-C4-C2	2.41	121.64	118.57
3	B	1372	NAP	C6N-N1N-C2N	-2.40	119.84	121.88
4	A	2002	X1H	C13-C11-C9	2.38	121.48	118.77
3	B	1372	NAP	O2A-PA-O1A	2.35	123.37	112.44
3	A	1372	NAP	C5A-C4A-N9A	2.33	108.34	105.81
3	B	1372	NAP	C3N-C7N-N7N	-2.28	114.92	117.74
4	A	2002	X1H	C9-C11-C8	-2.28	108.99	111.47
4	B	2002	X1H	C4-C7-C8	-2.27	126.70	130.17
3	B	1372	NAP	N9A-C8A-N7A	-2.26	110.73	113.94
3	B	1372	NAP	O4D-C4D-C5D	-2.26	102.10	109.33
3	B	1372	NAP	N3A-C4A-N9A	2.25	131.00	127.17
4	B	2001	X1H	C6-C4-C2	2.19	121.35	118.57
3	A	1372	NAP	C6N-N1N-C2N	-2.10	120.09	121.88
3	A	1372	NAP	P2B-O2B-C2B	-2.07	117.90	123.43
4	B	2001	X1H	C5-C6-C4	-2.06	118.59	120.80
4	B	2002	X1H	C6-C4-C2	2.06	121.19	118.57
3	A	1372	NAP	O2N-PN-O1N	2.01	121.79	112.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

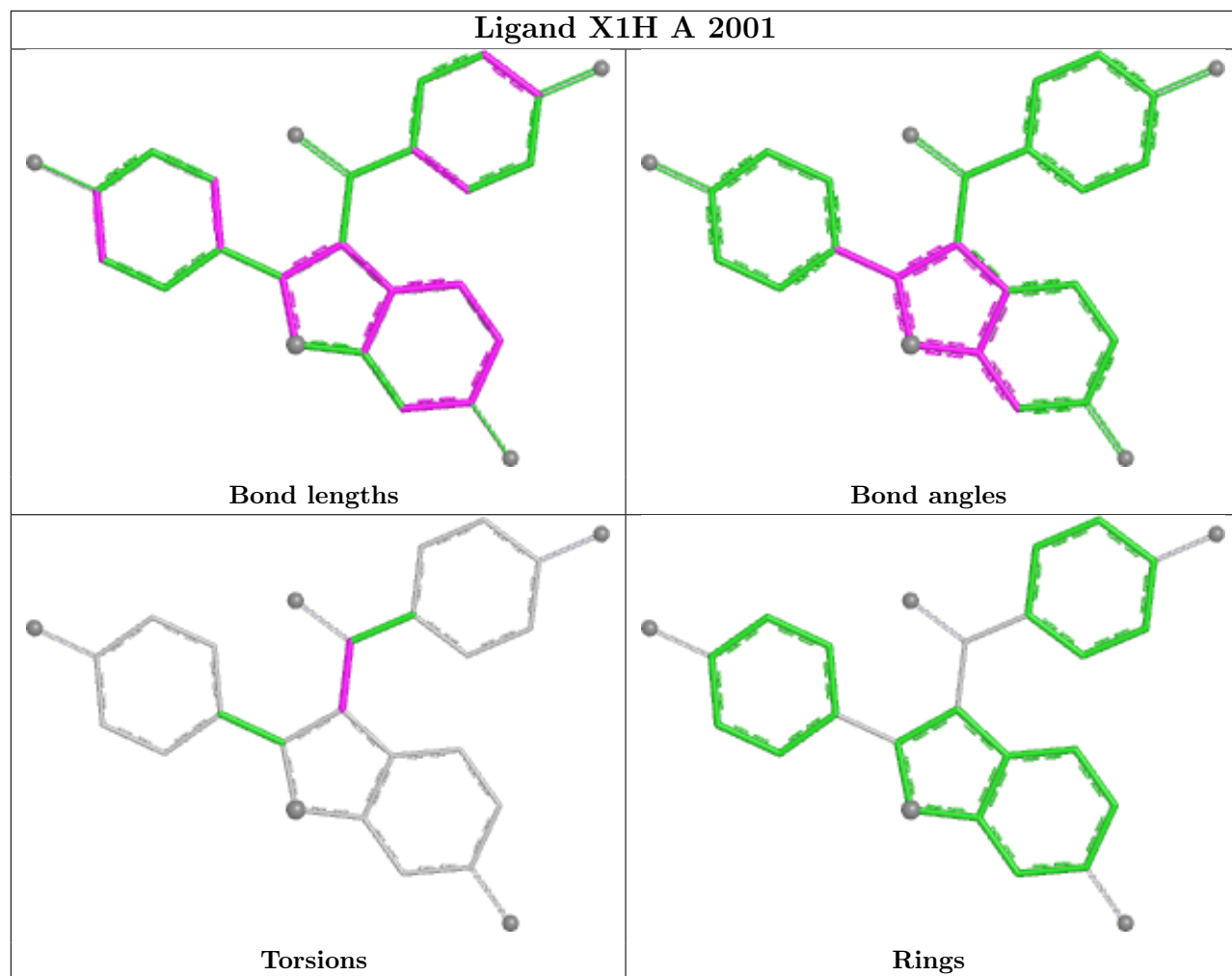
Mol	Chain	Res	Type	Atoms
4	A	2001	X1H	O1-C15-C8-C11
3	A	1372	NAP	PA-O3-PN-O2N
4	A	2001	X1H	O1-C15-C8-C7
3	A	1372	NAP	PA-O3-PN-O1N
3	B	1372	NAP	PA-O3-PN-O1N
3	B	1372	NAP	PA-O3-PN-O2N
4	A	2002	X1H	C19-C21-O3-C22
4	A	2002	X1H	C20-C21-O3-C22
3	A	1372	NAP	C4B-C5B-O5B-PA
2	A	1362	EDO	O1-C1-C2-O2
3	A	1372	NAP	O4B-C4B-C5B-O5B
3	B	1372	NAP	C4B-C5B-O5B-PA
3	A	1372	NAP	C1B-C2B-O2B-P2B
3	B	1372	NAP	O4B-C4B-C5B-O5B

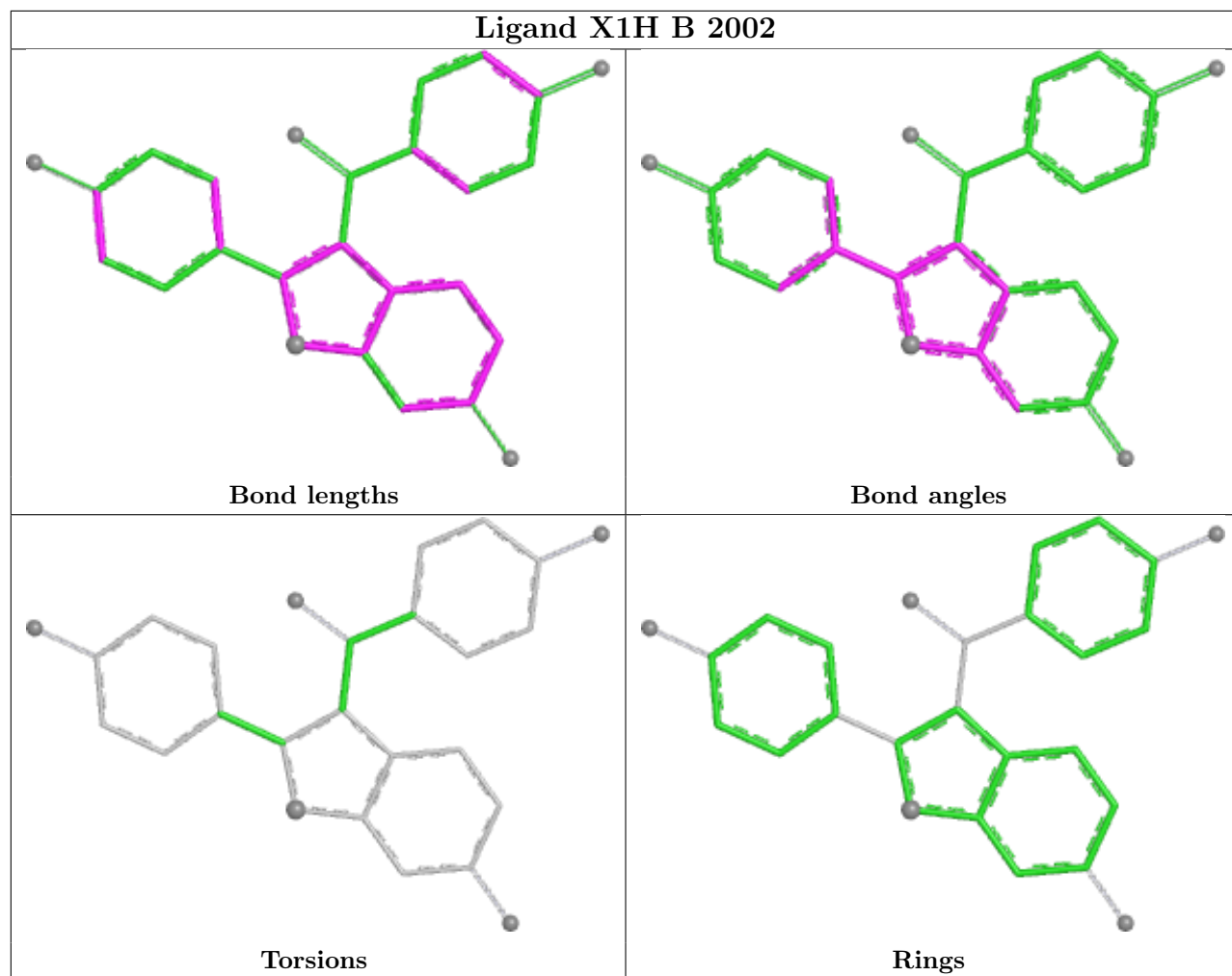
There are no ring outliers.

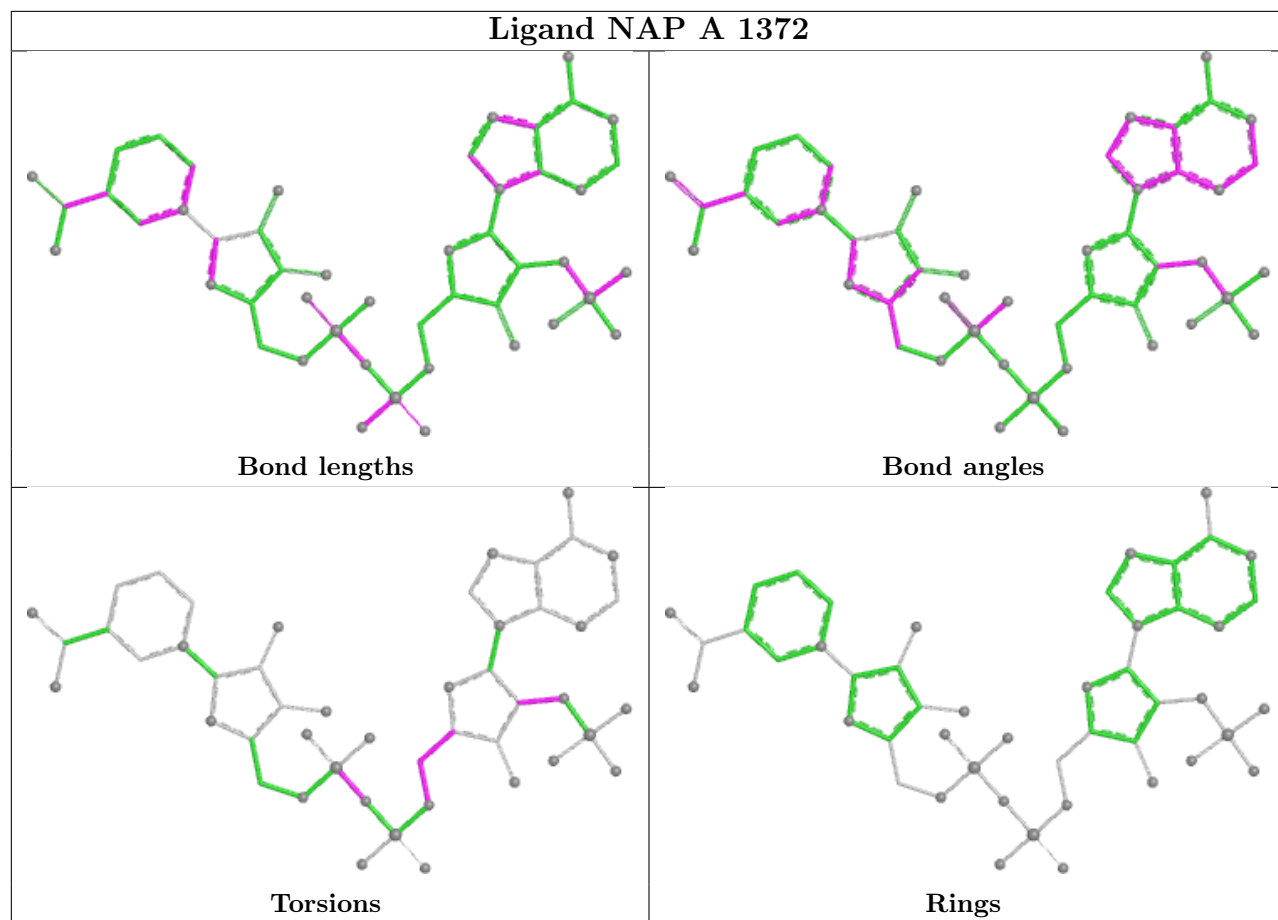
9 monomers are involved in 16 short contacts:

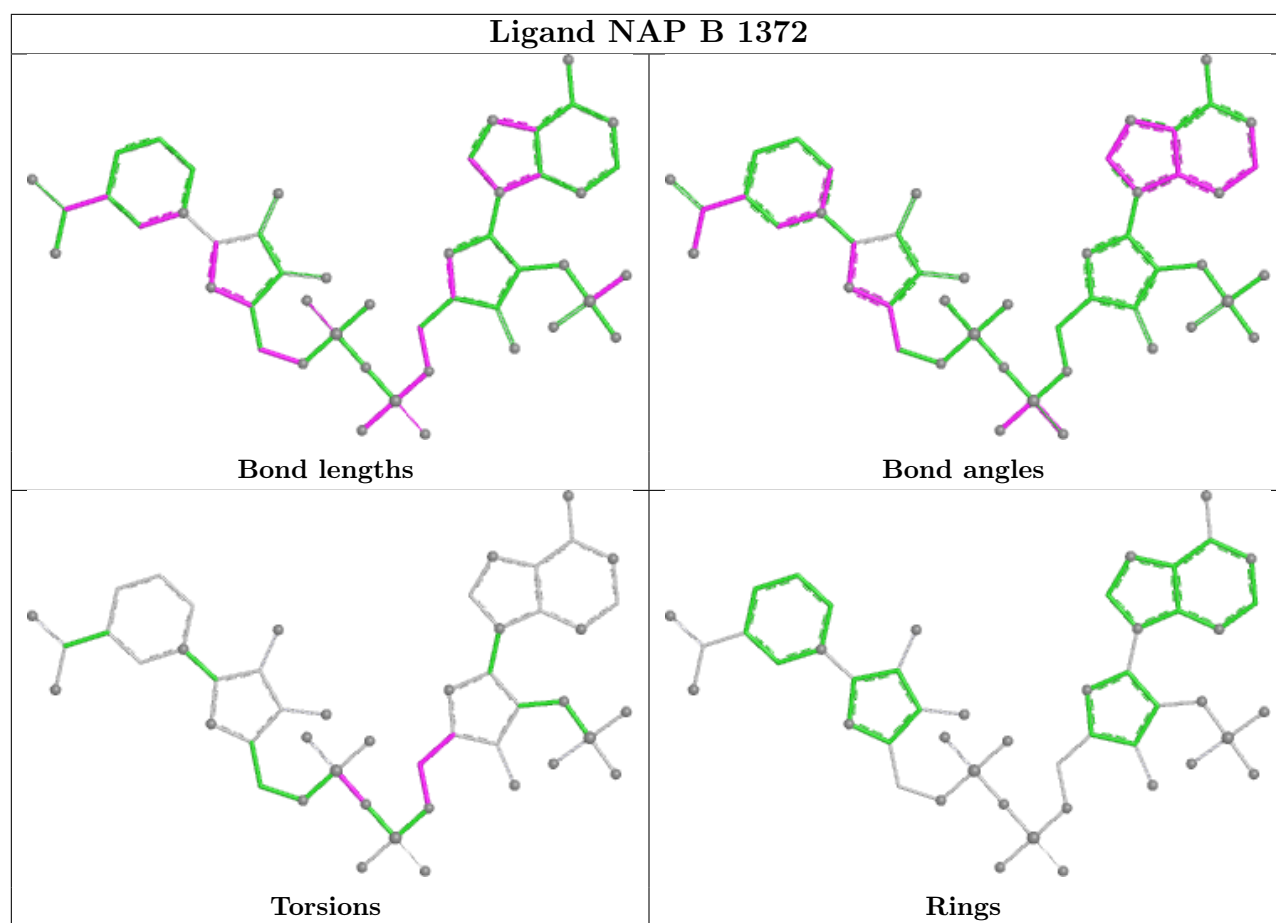
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	X1H	1	0
2	B	1362	EDO	1	0
4	B	2002	X1H	1	0
3	A	1372	NAP	5	0
2	A	1363	EDO	1	0
3	B	1372	NAP	3	0
2	A	1362	EDO	2	0
2	A	1364	EDO	2	0
4	A	2002	X1H	1	0

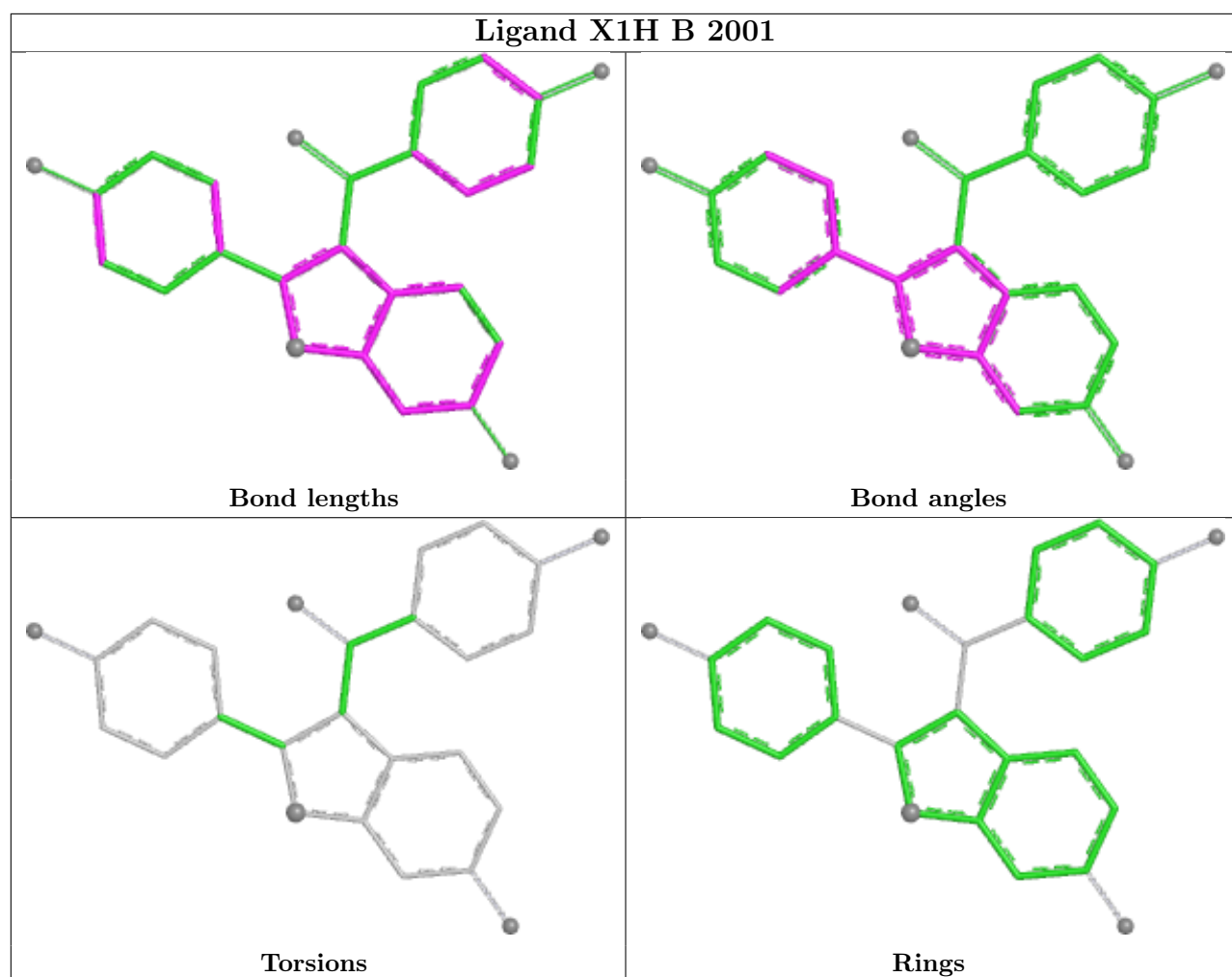
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

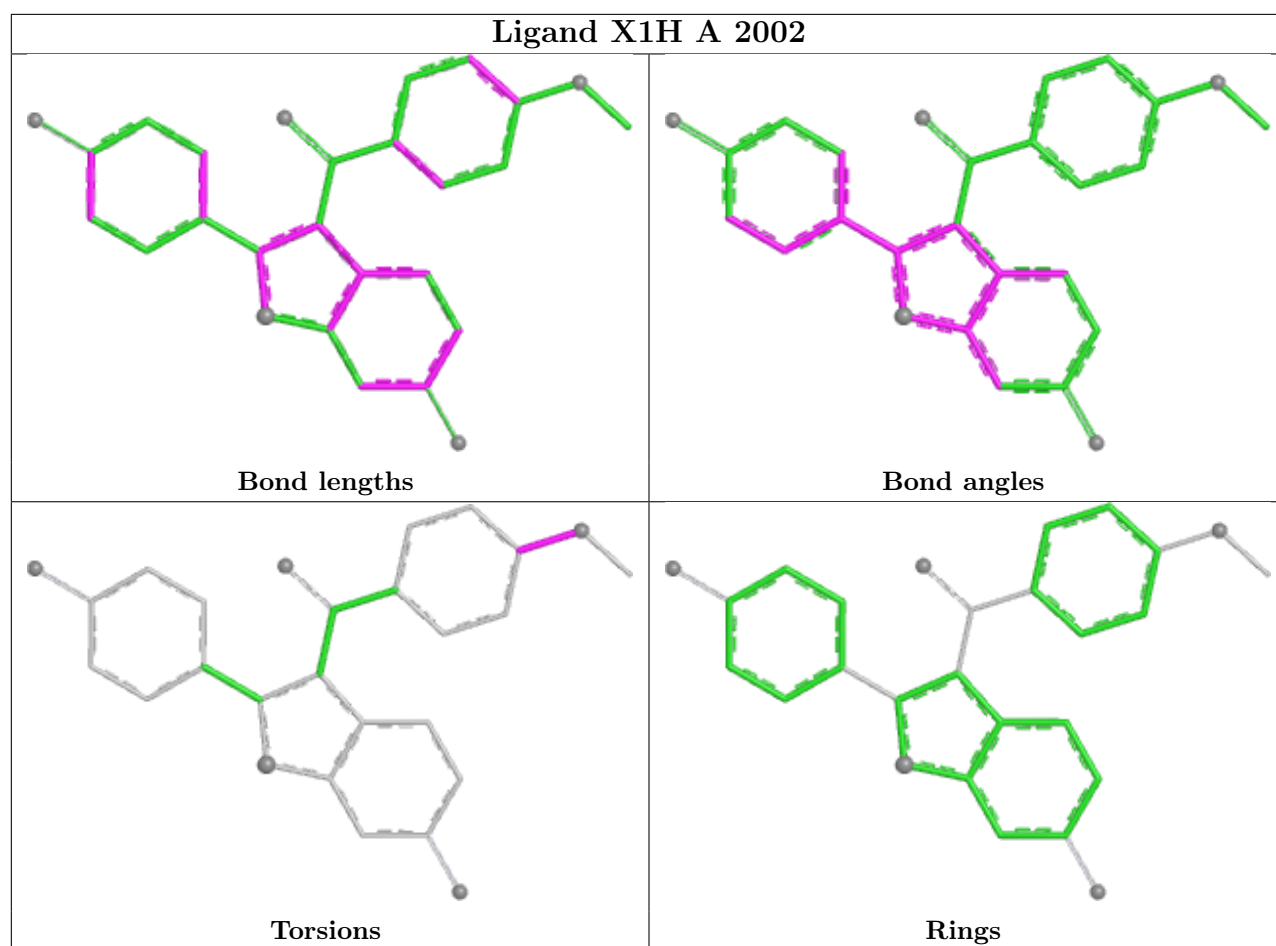












5.7 Other polymers [i](#)

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

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	340/362 (93%)	0.36	16 (4%) 36 42	7, 16, 37, 60	6 (1%)
1	B	339/362 (93%)	0.52	27 (7%) 18 22	8, 18, 39, 60	3 (0%)
All	All	679/724 (93%)	0.44	43 (6%) 26 30	7, 17, 37, 60	9 (1%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	LEU	5.4
1	B	328	LEU	4.8
1	B	330	PRO	4.5
1	A	328	LEU	4.5
1	A	50	LEU	4.3
1	B	81	VAL	3.6
1	B	53	ASP	3.6
1	A	330	PRO	3.5
1	A	311	LEU	3.5
1	B	361	PRO	3.5
1	B	311	LEU	3.4
1	A	43	SER	3.2
1	B	44	ARG	3.2
1	B	96	VAL	3.0
1	A	44	ARG	3.0
1	B	101	SER	3.0
1	A	312	GLU	3.0
1	B	100	LEU	2.9
1	B	117	PRO	2.8
1	B	103	SER	2.8
1	A	79	PRO	2.7
1	B	42	LEU	2.7
1	A	104	ALA	2.6
1	B	102	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	107	THR	2.6
1	B	105	ARG	2.6
1	B	45	ASP	2.6
1	A	22	SER	2.6
1	A	361	PRO	2.6
1	B	98	LEU	2.5
1	B	80	SER	2.4
1	A	327	ASP	2.4
1	A	317	GLY	2.3
1	B	106	TYR	2.3
1	B	77	TYR	2.3
1	B	130	ILE	2.3
1	A	105	ARG	2.2
1	A	45	ASP	2.1
1	A	81	VAL	2.1
1	B	51	PRO	2.1
1	B	317	GLY	2.0
1	B	181	MET	2.0
1	B	25	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

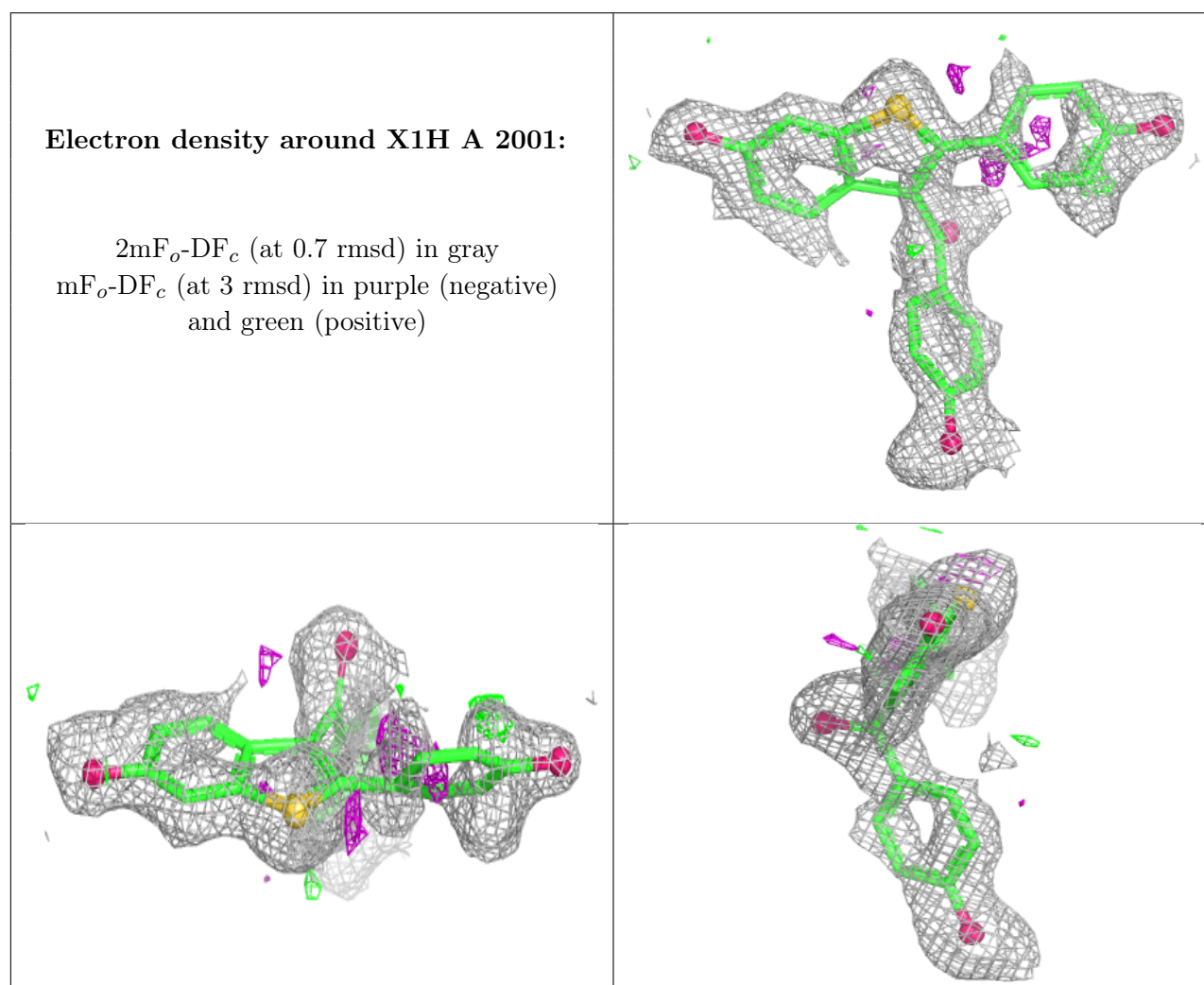
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	B	1362	4/4	0.82	0.19	21,30,30,41	0
2	EDO	A	1363	4/4	0.83	0.17	36,36,40,48	0
2	EDO	A	1364	4/4	0.86	0.16	29,33,35,42	0
4	X1H	A	2001	26/27	0.88	0.14	14,32,41,47	0

Continued on next page...

Continued from previous page...

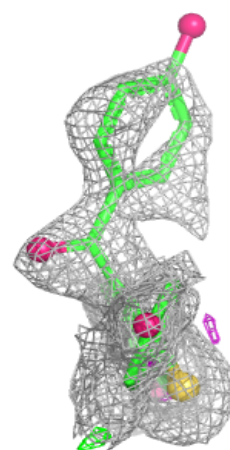
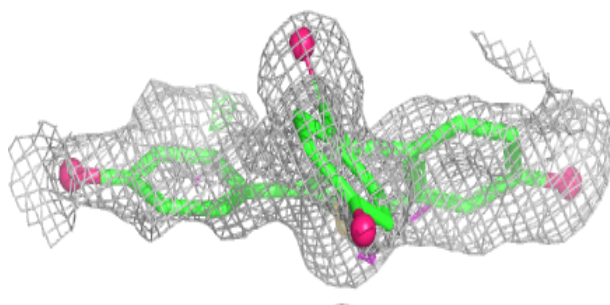
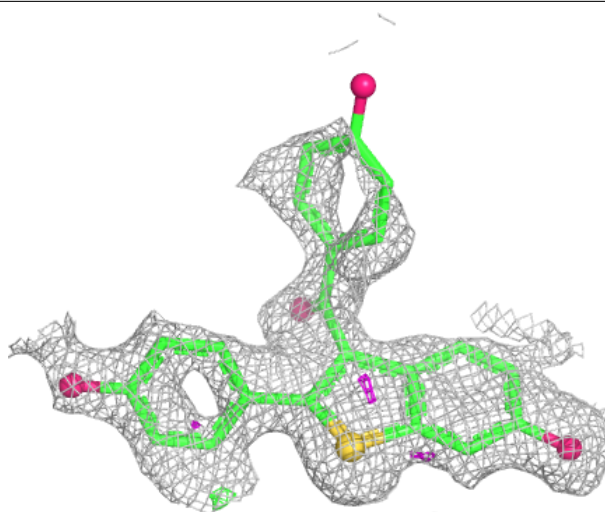
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	X1H	B	2001	26/27	0.90	0.13	13,36,43,51	0
4	X1H	B	2002	26/27	0.91	0.13	16,30,54,60	0
4	X1H	A	2002	27/27	0.92	0.10	6,20,32,39	0
2	EDO	A	1362	4/4	0.94	0.09	12,12,20,21	0
3	NAP	A	1372	48/48	0.97	0.07	1,13,28,39	0
3	NAP	B	1372	48/48	0.97	0.07	3,14,27,53	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.



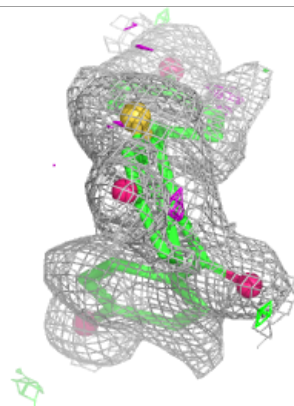
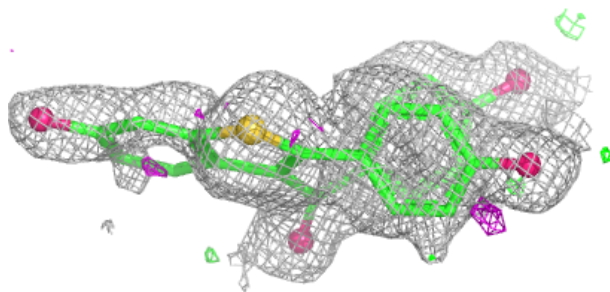
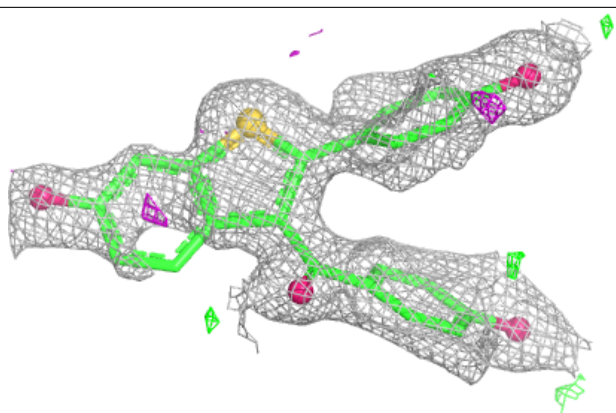
Electron density around X1H B 2001:

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

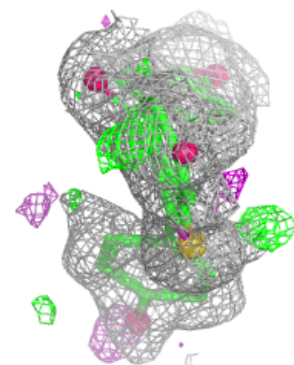
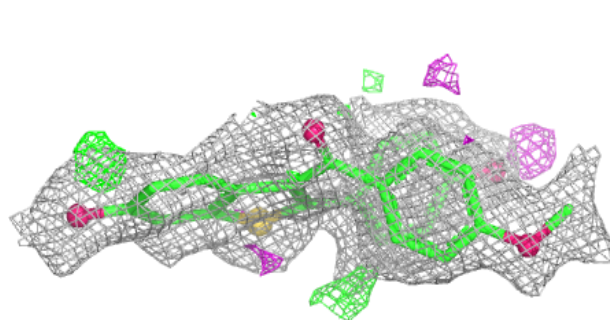
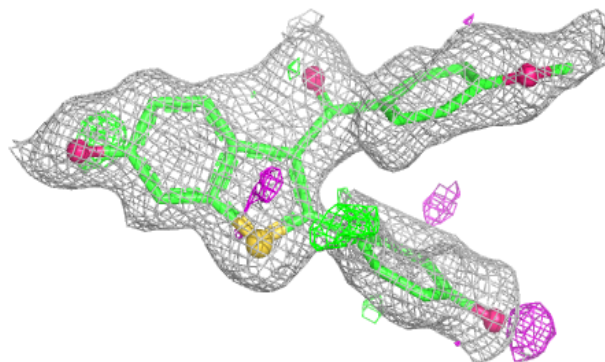


Electron density around X1H B 2002:

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

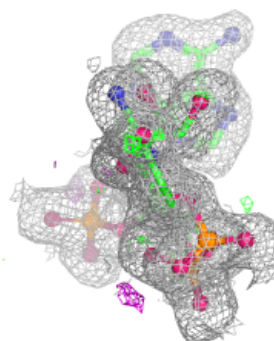
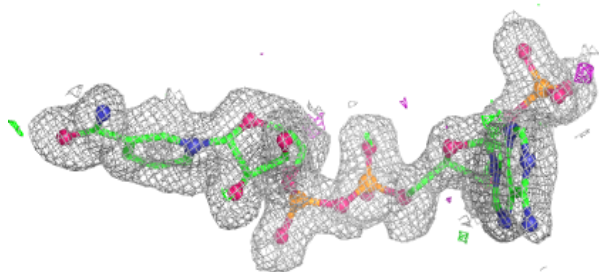
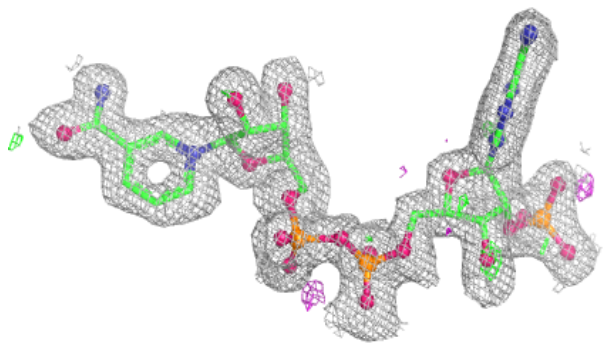
**Electron density around X1H A 2002:**

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

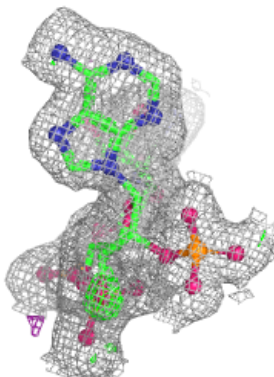
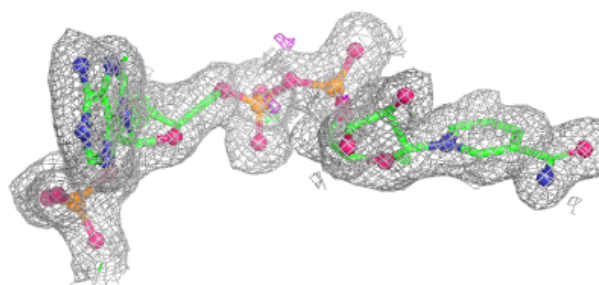
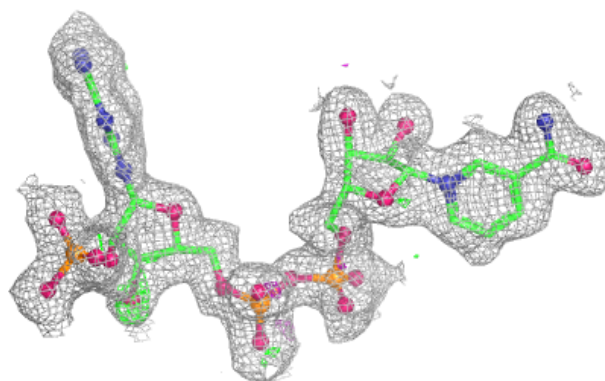


Electron density around NAP A 1372:

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

**Electron density around NAP B 1372:**

$2mF_o-DF_c$ (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.