



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:32 PM UTC

PDB ID : 2OPB / pdb_00002opb
Title : Structure of K57A hPNMT with inhibitor 3-fluoromethyl-7-thiomorpholinosu
lfonamide-THIQ and AdoHcy
Authors : Drinkwater, N.; Martin, J.L.
Deposited on : 2007-01-28
Resolution : 2.80 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

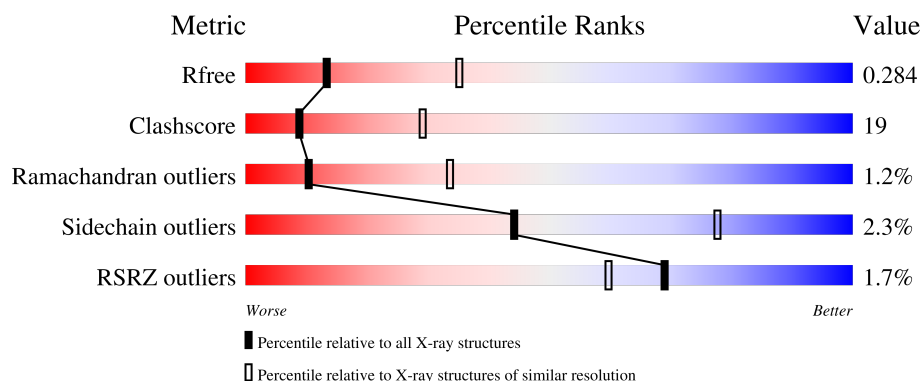
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	289	 2% 51% 36% 11%
1	B	289	 0% 56% 34% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4263 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.

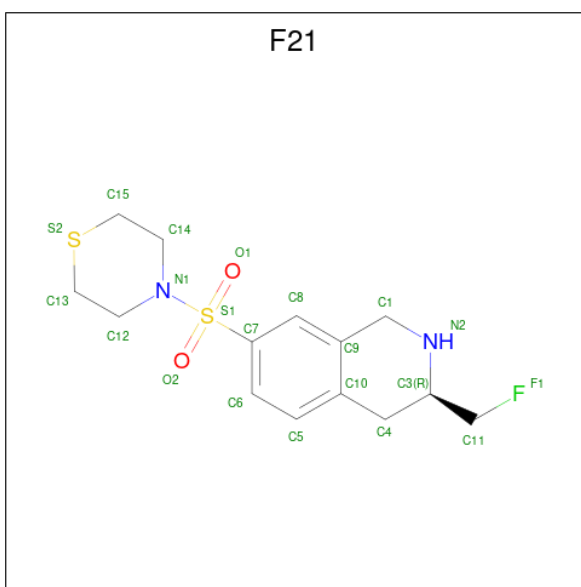
- Molecule 1 is a protein called Phenylethanolamine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2012	1277	357	369	9			
1	B	268	Total	C	N	O	S	0	0	0
			2079	1317	369	384	9			

There are 16 discrepancies between the modelled and reference sequences:

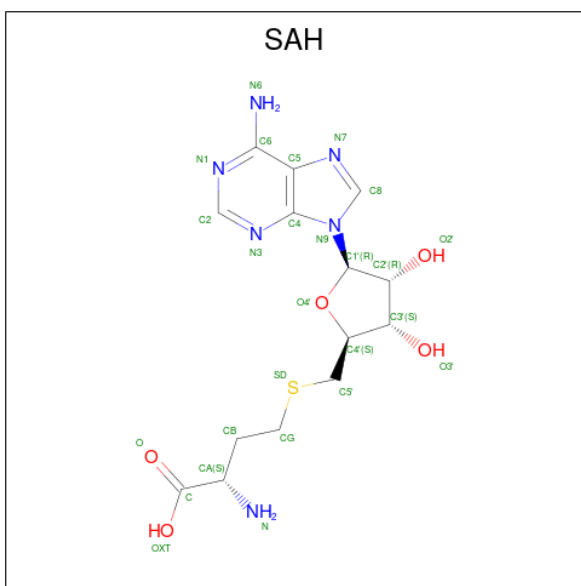
Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	LYS	modified residue	UNP P11086
A	283	GLU	-	expression tag	UNP P11086
A	284	HIS	-	expression tag	UNP P11086
A	285	HIS	-	expression tag	UNP P11086
A	286	HIS	-	expression tag	UNP P11086
A	287	HIS	-	expression tag	UNP P11086
A	288	HIS	-	expression tag	UNP P11086
A	289	HIS	-	expression tag	UNP P11086
B	57	ALA	LYS	modified residue	UNP P11086
B	283	GLU	-	expression tag	UNP P11086
B	284	HIS	-	expression tag	UNP P11086
B	285	HIS	-	expression tag	UNP P11086
B	286	HIS	-	expression tag	UNP P11086
B	287	HIS	-	expression tag	UNP P11086
B	288	HIS	-	expression tag	UNP P11086
B	289	HIS	-	expression tag	UNP P11086

- Molecule 2 is (3R)-3-(FLUOROMETHYL)-7-(THIOMORPHOLIN-4-YLSULFONYL)-1,2,3,4-TETRAHYDROISOQUINOLINE (CCD ID: F21) (formula: C₁₄H₁₉FN₂O₂S₂).



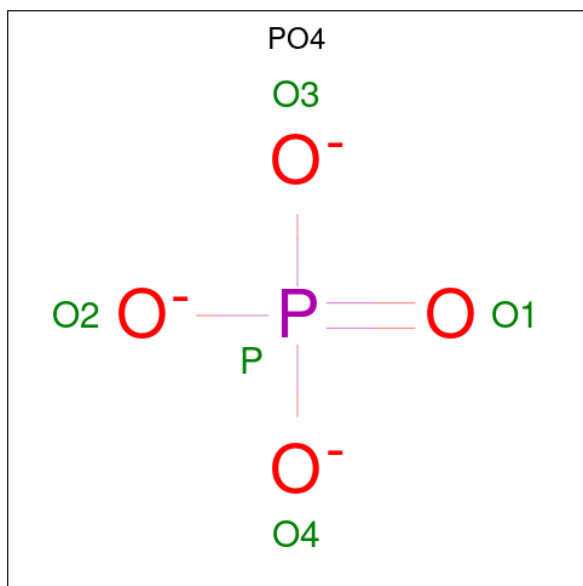
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			21	14	1	2	2	2		
2	B	1	Total	C	F	N	O	S	0	0
			21	14	1	2	2	2		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

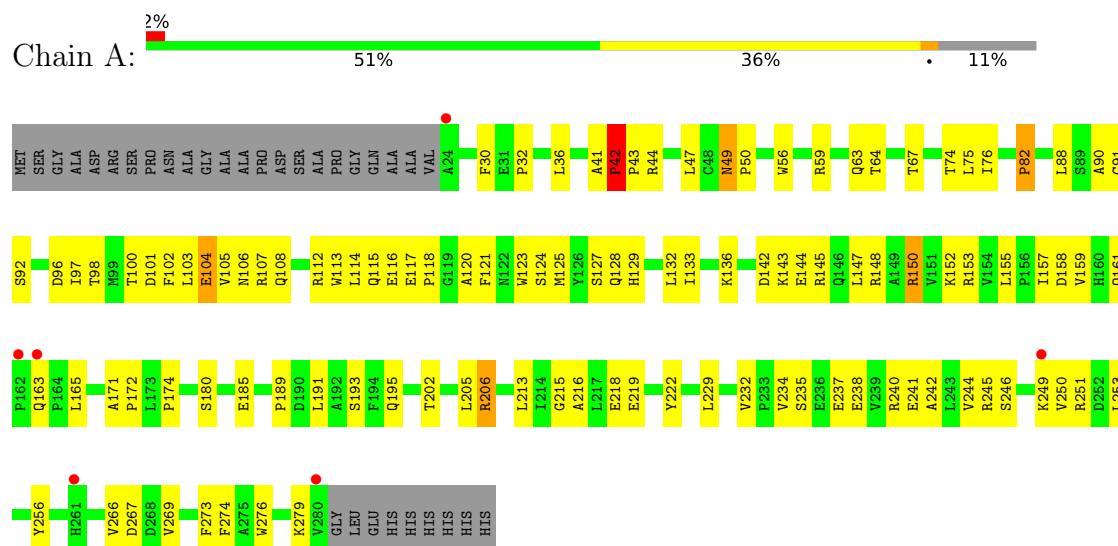
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	34	Total	O	0	0
			34	34		

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: Phenylethanolamine N-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.42Å 94.42Å 187.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.40 – 2.80 54.40 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (54.40-2.80) 96.6 (54.40-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.277 0.237 , 0.284	Depositor DCC
R_{free} test set	1054 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4263	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: PO4, SAH, F21

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	0.50	0/2063	1.05	9/2809 (0.3%)
1	B	0.50	0/2132	1.04	12/2904 (0.4%)
All	All	0.50	0/4195	1.04	21/5713 (0.4%)

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	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	SER	CA-C-N	9.94	129.31	118.97
1	B	169	SER	C-N-CA	9.94	129.31	118.97
1	A	49	ASN	CA-C-N	8.95	129.52	119.32
1	A	49	ASN	C-N-CA	8.95	129.52	119.32
1	A	163	GLN	CA-C-N	8.43	130.38	119.84
1	A	163	GLN	C-N-CA	8.43	130.38	119.84
1	A	42	PRO	CB-CA-C	6.74	119.14	110.92
1	B	227	ALA	N-CA-C	6.53	119.69	109.96
1	A	266	VAL	N-CA-C	-6.49	103.49	113.16
1	B	140	TRP	N-CA-C	6.30	118.95	111.71
1	B	266	VAL	N-CA-C	-6.24	104.21	113.39
1	A	155	LEU	N-CA-C	6.24	118.90	110.29
1	B	28	GLN	N-CA-C	-5.79	105.98	113.16
1	B	166	GLY	N-CA-C	-5.58	104.55	112.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	GLY	N-CA-C	-5.49	107.69	115.43
1	A	136	LYS	N-CA-C	-5.44	106.23	112.92
1	B	264	THR	N-CA-C	5.41	118.99	112.93
1	B	229	LEU	N-CA-C	5.33	118.36	110.48
1	B	142	ASP	N-CA-C	-5.29	105.69	111.82
1	A	120	ALA	N-CA-C	-5.23	103.79	110.53
1	B	83	THR	N-CA-C	5.13	117.95	109.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	PRO	Mainchain

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	2012	0	1975	81	0
1	B	2079	0	2037	74	0
2	A	21	0	19	2	0
2	B	21	0	19	1	0
3	A	26	0	19	1	0
3	B	26	0	19	3	0
4	B	5	0	0	0	0
5	A	39	0	0	2	0
5	B	34	0	0	2	0
All	All	4263	0	4088	154	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 19.

All (154) 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:115:GLN:HB2	1:A:117:GLU:HG3	1.54	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:THR:HG22	1:A:96:ASP:HB3	1.54	0.89
1:B:29:ARG:HH21	1:B:226:GLU:HB3	1.39	0.86
1:A:237:GLU:O	1:A:241:GLU:HG3	1.75	0.86
1:A:128:GLN:HB3	1:B:128:GLN:OE1	1.76	0.85
1:A:124:SER:O	1:A:128:GLN:HG3	1.77	0.84
1:B:235:SER:OG	1:B:238:GLU:HG3	1.78	0.82
1:B:195:GLN:HE22	1:B:242:ALA:HA	1.42	0.82
1:A:129:HIS:ND1	5:A:4040:HOH:O	2.17	0.76
1:A:150:ARG:HG2	1:A:150:ARG:HH11	1.50	0.74
1:A:59:ARG:O	1:A:63:GLN:HG3	1.89	0.72
1:A:150:ARG:HG2	1:A:150:ARG:NH1	2.06	0.71
1:A:235:SER:OG	1:A:238:GLU:HG3	1.92	0.70
1:B:59:ARG:O	1:B:63:GLN:HG3	1.93	0.69
1:B:219:GLU:OE1	1:B:269:VAL:HB	1.93	0.68
1:A:103:LEU:HB3	1:A:105:VAL:HG22	1.76	0.67
1:B:128:GLN:HE21	1:B:128:GLN:HA	1.61	0.66
1:A:142:ASP:OD1	1:A:145:ARG:NH2	2.30	0.64
1:A:88:LEU:O	1:A:143:LYS:HE3	1.98	0.64
1:A:103:LEU:HB3	1:A:105:VAL:CG2	2.28	0.63
1:A:125:MET:HE1	1:B:141:GLN:NE2	2.14	0.62
1:B:207:PRO:HB3	1:B:281:GLY:HA3	1.81	0.62
1:A:32:PRO:HG3	1:A:106:ASN:ND2	2.14	0.61
1:A:98:THR:HG23	1:A:153:ARG:HG3	1.81	0.61
1:A:159:VAL:HG22	3:A:3001:SAH:N1	2.16	0.61
1:B:36:LEU:HD21	1:B:82:PRO:HG2	1.83	0.60
1:A:195:GLN:HE22	1:A:242:ALA:HA	1.68	0.59
2:A:4001:F21:H122	2:A:4001:F21:H6	1.85	0.59
1:A:75:LEU:HD23	1:A:76:ILE:N	2.18	0.58
1:A:74:THR:HG21	1:A:172:PRO:HB2	1.85	0.57
1:B:192:ALA:HB1	1:B:196:ARG:HH12	1.69	0.57
1:B:196:ARG:HH11	1:B:196:ARG:HG3	1.70	0.56
1:B:147:LEU:O	1:B:151:VAL:HG23	2.05	0.56
1:B:158:ASP:O	1:B:164:PRO:HA	2.05	0.56
1:B:207:PRO:CB	1:B:281:GLY:HA3	2.36	0.55
1:A:41:ALA:O	1:A:42:PRO:C	2.48	0.55
1:A:113:TRP:CH2	1:A:147:LEU:HD23	2.41	0.55
1:B:186:ALA:HA	1:B:231:VAL:HG13	1.89	0.55
1:B:223:LEU:HD23	1:B:228:ARG:HA	1.89	0.55
1:A:232:VAL:O	1:A:234:VAL:HG13	2.05	0.54
1:B:185:GLU:OE2	1:B:216:ALA:N	2.37	0.54
1:A:56:TRP:CE2	1:A:256:TYR:HB2	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ARG:HH21	1:B:226:GLU:CB	2.15	0.54
1:A:241:GLU:O	1:A:245:ARG:HG3	2.07	0.54
1:A:44:ARG:HD3	2:A:4001:F21:O1	2.08	0.54
1:B:74:THR:HG21	1:B:172:PRO:HB2	1.90	0.53
1:B:38:ASN:HB3	1:B:266:VAL:HG11	1.89	0.53
1:A:64:THR:O	1:A:67:THR:HG23	2.09	0.52
1:A:189:PRO:HD2	1:A:193:SER:OG	2.09	0.52
1:A:97:ILE:HD12	1:A:150:ARG:HB3	1.90	0.52
1:A:222:TYR:CE2	1:A:229:LEU:HB2	2.44	0.52
1:A:115:GLN:O	1:A:116:GLU:C	2.53	0.52
1:A:165:LEU:HB2	5:A:4015:HOH:O	2.10	0.52
1:B:75:LEU:HG	1:B:76:ILE:N	2.25	0.52
1:B:152:LYS:O	1:B:153:ARG:HB3	2.10	0.51
1:A:75:LEU:HD23	1:A:75:LEU:C	2.34	0.51
1:A:129:HIS:O	1:A:133:ILE:HG13	2.10	0.51
1:A:36:LEU:HD21	1:A:82:PRO:HG2	1.92	0.51
1:A:158:ASP:HB3	1:A:161:GLN:HG2	1.93	0.51
1:A:144:GLU:O	1:A:148:ARG:HG3	2.11	0.51
1:B:83:THR:HA	1:B:123:TRP:CZ2	2.45	0.51
1:A:47:LEU:HB3	1:A:129:HIS:CE1	2.46	0.50
1:A:249:LYS:O	1:A:249:LYS:HG2	2.11	0.50
1:A:47:LEU:O	1:A:129:HIS:CE1	2.65	0.50
1:A:202:THR:O	1:A:279:LYS:NZ	2.37	0.50
1:A:251:ARG:HB2	1:A:276:TRP:O	2.12	0.50
1:B:53:VAL:HB	1:B:256:TYR:CE2	2.47	0.49
1:B:78:ILE:HB	1:B:180:SER:HB2	1.95	0.49
1:A:98:THR:HG23	1:A:153:ARG:CG	2.42	0.49
1:B:100:THR:O	1:B:101:ASP:HB2	2.13	0.49
1:B:195:GLN:NE2	1:B:242:ALA:HA	2.20	0.49
1:A:276:TRP:C	1:A:276:TRP:CD1	2.90	0.49
1:B:38:ASN:HB3	1:B:266:VAL:CG1	2.43	0.49
1:B:40:TYR:OH	1:B:85:TYR:CE2	2.66	0.49
1:A:253:LEU:HD12	1:A:274:PHE:O	2.13	0.49
1:A:32:PRO:HG3	1:A:106:ASN:HD21	1.77	0.48
1:A:150:ARG:HH11	1:A:150:ARG:CG	2.24	0.48
1:B:215:GLY:HA3	1:B:273:PHE:CE2	2.48	0.48
1:B:40:TYR:OH	3:B:3002:SAH:OXT	2.24	0.48
1:A:267:ASP:OD1	1:A:269:VAL:HG12	2.14	0.48
1:B:73:ARG:HG3	1:B:95:GLU:OE2	2.14	0.47
1:B:227:ALA:HB1	1:B:229:LEU:HD11	1.96	0.47
1:B:253:LEU:HD13	1:B:275:ALA:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:O	1:A:148:ARG:HD3	2.15	0.47
1:A:174:PRO:HG2	1:A:206:ARG:HB2	1.97	0.47
1:A:47:LEU:O	1:A:129:HIS:HE1	1.97	0.46
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.80	0.46
1:A:124:SER:O	1:A:128:GLN:CG	2.57	0.46
1:B:75:LEU:HD11	1:B:179:VAL:HG23	1.98	0.46
2:B:4002:F21:H141	2:B:4002:F21:H6	1.95	0.46
1:B:106:ASN:HD22	1:B:106:ASN:HA	1.53	0.46
1:A:104:GLU:OE1	1:A:108:GLN:OE1	2.33	0.46
1:A:171:ALA:HA	1:A:172:PRO:HD3	1.80	0.46
1:B:157:ILE:HG13	1:B:164:PRO:O	2.15	0.46
1:A:174:PRO:CG	1:A:206:ARG:HB2	2.46	0.46
1:B:19:GLY:O	1:B:22:ALA:HB3	2.16	0.46
1:A:88:LEU:HD13	1:A:127:SER:HA	1.97	0.45
1:A:100:THR:O	1:A:101:ASP:HB2	2.15	0.45
1:B:115:GLN:HB2	1:B:117:GLU:HG3	1.98	0.45
1:A:215:GLY:HA3	1:A:273:PHE:CE2	2.52	0.45
1:A:218:GLU:HA	1:A:218:GLU:OE2	2.16	0.45
1:B:56:TRP:CE2	1:B:256:TYR:HB2	2.51	0.45
1:B:35:TYR:CE1	1:B:39:ASN:ND2	2.84	0.45
1:B:91:CYS:HB3	1:B:147:LEU:HD13	1.98	0.45
1:B:159:VAL:HG13	3:B:3002:SAH:H2	1.97	0.45
1:A:30:PHE:HB3	1:A:103:LEU:CD1	2.47	0.45
1:A:222:TYR:CB	1:A:267:ASP:HB3	2.46	0.45
1:A:49:ASN:HA	1:A:50:PRO:HD3	1.69	0.45
1:A:90:ALA:O	1:A:92:SER:N	2.49	0.45
1:B:65:PHE:CE1	1:B:90:ALA:HB2	2.51	0.45
1:A:132:LEU:HG	1:B:137:GLY:HA2	1.99	0.44
1:A:121:PHE:HD2	1:A:123:TRP:CE2	2.35	0.44
1:B:29:ARG:NH2	1:B:226:GLU:HB3	2.21	0.44
1:B:40:TYR:OH	1:B:85:TYR:HE2	2.01	0.44
1:B:128:GLN:HE21	1:B:128:GLN:CA	2.28	0.44
1:A:229:LEU:HD22	1:A:229:LEU:N	2.32	0.44
1:B:188:SER:HA	1:B:189:PRO:HD3	1.84	0.44
1:B:228:ARG:NH2	5:B:4030:HOH:O	2.51	0.44
1:B:196:ARG:HG3	1:B:196:ARG:NH1	2.32	0.44
1:B:79:GLY:O	3:B:3002:SAH:N	2.50	0.43
1:B:158:ASP:OD1	1:B:160:HIS:HB2	2.18	0.43
1:B:202:THR:O	1:B:202:THR:HG22	2.18	0.43
1:A:117:GLU:HB3	1:A:118:PRO:CD	2.49	0.43
1:B:85:TYR:CG	1:B:86:GLN:N	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:OG1	1:B:153:ARG:NH1	2.50	0.43
1:B:23:VAL:HG12	1:B:24:ALA:N	2.34	0.43
1:B:146:GLN:O	1:B:150:ARG:HG3	2.19	0.42
1:B:276:TRP:CD1	1:B:276:TRP:C	2.97	0.42
1:A:63:GLN:O	1:A:67:THR:HG23	2.19	0.42
1:A:185:GLU:OE2	1:A:216:ALA:N	2.43	0.42
1:A:104:GLU:HB2	1:A:107:ARG:NH2	2.34	0.42
1:A:102:PHE:HD1	1:A:157:ILE:O	2.02	0.42
1:B:74:THR:OG1	1:B:175:ALA:HA	2.19	0.42
1:A:96:ASP:OD1	1:A:152:LYS:HG3	2.19	0.42
1:A:145:ARG:HH11	1:A:145:ARG:HG3	1.85	0.42
1:B:66:ALA:C	1:B:68:GLY:N	2.77	0.42
1:B:32:PRO:HG3	1:B:106:ASN:ND2	2.35	0.42
1:B:185:GLU:HG2	1:B:186:ALA:N	2.35	0.42
1:B:261:HIS:ND1	5:B:4013:HOH:O	2.37	0.42
1:B:229:LEU:N	1:B:229:LEU:HD12	2.35	0.42
1:A:219:GLU:OE1	1:A:269:VAL:HB	2.20	0.41
1:B:80:SER:HB2	1:B:100:THR:O	2.19	0.41
1:B:221:TRP:HA	1:B:229:LEU:O	2.21	0.41
1:B:170:PRO:O	1:B:171:ALA:C	2.64	0.41
1:A:96:ASP:OD2	1:A:172:PRO:HG2	2.21	0.41
1:B:65:PHE:CZ	1:B:90:ALA:HB2	2.56	0.41
1:B:258:MET:HA	1:B:259:PRO:HD3	1.97	0.41
1:A:180:SER:HB3	1:A:213:LEU:HD12	2.03	0.40
1:B:201:ILE:HG13	1:B:202:THR:N	2.34	0.40
1:A:74:THR:HG21	1:A:172:PRO:CB	2.50	0.40
1:A:205:LEU:HD23	1:A:279:LYS:HB2	2.03	0.40
1:A:240:ARG:O	1:A:244:VAL:HG23	2.22	0.40
1:B:67:THR:C	1:B:69:GLU:H	2.29	0.40
1:B:140:TRP:O	1:B:143:LYS:HB3	2.21	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	255/289 (88%)	235 (92%)	16 (6%)	4 (2%)	7	27
1	B	266/289 (92%)	248 (93%)	16 (6%)	2 (1%)	16	44
All	All	521/578 (90%)	483 (93%)	32 (6%)	6 (1%)	10	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	CYS
1	A	42	PRO
1	B	120	ALA
1	A	82	PRO
1	B	153	ARG
1	A	250	VAL

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	211/232 (91%)	205 (97%)	6 (3%)	38	73
1	B	217/232 (94%)	213 (98%)	4 (2%)	51	82
All	All	428/464 (92%)	418 (98%)	10 (2%)	44	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	PRO
1	A	104	GLU
1	A	150	ARG
1	A	191	LEU
1	A	206	ARG
1	A	246	SER
1	B	106	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	128	GLN
1	B	136	LYS
1	B	237	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	106	ASN
1	A	108	GLN
1	A	129	HIS
1	A	195	GLN
1	A	210	HIS
1	A	278	GLN
1	B	39	ASN
1	B	106	ASN
1	B	108	GLN
1	B	128	GLN
1	B	146	GLN
1	B	160	HIS
1	B	163	GLN
1	B	195	GLN
1	B	263	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](#)

5 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$
2	F21	A	4001	-	22,23,23	1.56	1 (4%)	29,33,33	2.93	9 (31%)
4	PO4	B	290	-	4,4,4	2.70	3 (75%)	6,6,6	0.47	0
3	SAH	A	3001	-	27,28,28	0.93	1 (3%)	36,40,40	0.72	0
3	SAH	B	3002	-	27,28,28	0.94	1 (3%)	36,40,40	0.69	1 (2%)
2	F21	B	4002	-	22,23,23	1.58	1 (4%)	29,33,33	2.94	10 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	A	3001	-	-	6/15/31/31	0/3/3/3
2	F21	A	4001	-	-	8/12/31/31	0/3/3/3
3	SAH	B	3002	-	-	4/15/31/31	0/3/3/3
2	F21	B	4002	-	-	4/12/31/31	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	F21	O1-S1	6.53	1.50	1.43
2	B	4002	F21	O1-S1	6.53	1.50	1.43
3	B	3002	SAH	C8-N9	3.74	1.43	1.37
3	A	3001	SAH	C8-N9	3.43	1.43	1.37
4	B	290	PO4	P-O4	-3.04	1.45	1.54
4	B	290	PO4	P-O3	-2.90	1.46	1.54
4	B	290	PO4	P-O2	-2.89	1.46	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4001	F21	C7-S1-N1	8.32	117.31	107.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4002	F21	C7-S1-N1	8.29	117.28	107.28
2	A	4001	F21	O1-S1-O2	-6.62	109.26	119.59
2	B	4002	F21	O1-S1-O2	-6.53	109.40	119.59
2	A	4001	F21	C14-C15-S2	-5.20	106.42	112.46
2	B	4002	F21	C12-C13-S2	-5.06	106.59	112.46
2	A	4001	F21	C14-N1-S1	-4.82	108.10	117.06
2	B	4002	F21	C14-C15-S2	-4.80	106.89	112.46
2	A	4001	F21	C15-S2-C13	4.62	105.39	97.58
2	B	4002	F21	C14-N1-S1	-4.46	108.76	117.06
2	A	4001	F21	C12-C13-S2	-4.36	107.40	112.46
2	B	4002	F21	C15-S2-C13	4.17	104.63	97.58
2	B	4002	F21	C12-N1-S1	-4.00	109.61	117.06
2	B	4002	F21	C6-C7-S1	3.44	123.15	119.73
2	A	4001	F21	C12-N1-S1	-3.38	110.76	117.06
2	A	4001	F21	C6-C7-S1	3.22	122.93	119.73
2	B	4002	F21	C8-C7-S1	-2.65	116.41	119.30
2	B	4002	F21	C14-N1-C12	2.38	114.86	112.12
2	A	4001	F21	C14-N1-C12	2.32	114.79	112.12
3	B	3002	SAH	C4-C5-N7	2.08	112.96	110.58

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4001	F21	C6-C7-S1-N1
2	A	4001	F21	C8-C7-S1-N1
2	B	4002	F21	C6-C7-S1-N1
2	B	4002	F21	C8-C7-S1-N1
2	A	4001	F21	C12-N1-S1-O2
3	B	3002	SAH	C2'-C1'-N9-C8
2	B	4002	F21	C8-C7-S1-O1
2	B	4002	F21	C6-C7-S1-O1
3	A	3001	SAH	C2'-C1'-N9-C8
2	A	4001	F21	C8-C7-S1-O1
2	A	4001	F21	C6-C7-S1-O1
3	B	3002	SAH	CB-CG-SD-C5'
3	A	3001	SAH	OXT-C-CA-CB
3	A	3001	SAH	O-C-CA-CB
3	A	3001	SAH	C2'-C1'-N9-C4
3	B	3002	SAH	C2'-C1'-N9-C4
3	A	3001	SAH	CB-CG-SD-C5'
2	A	4001	F21	C6-C7-S1-O2

Continued on next page...

Continued from previous page...

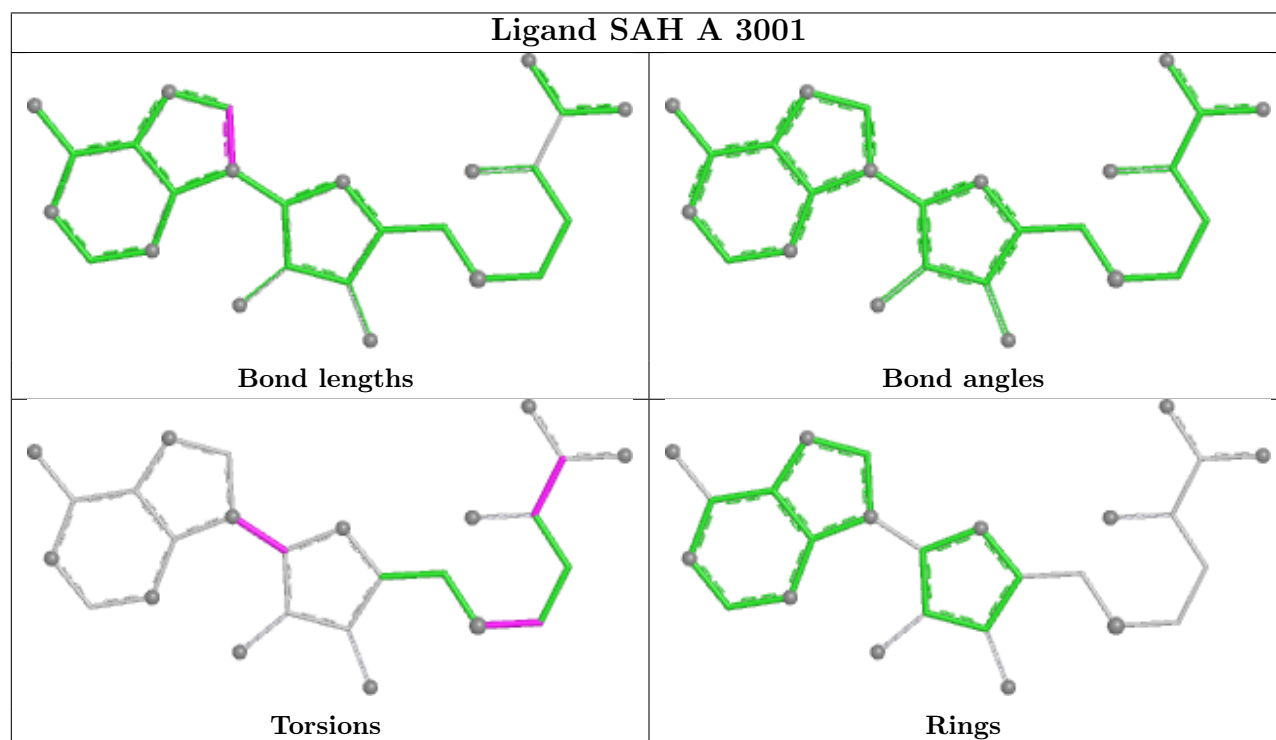
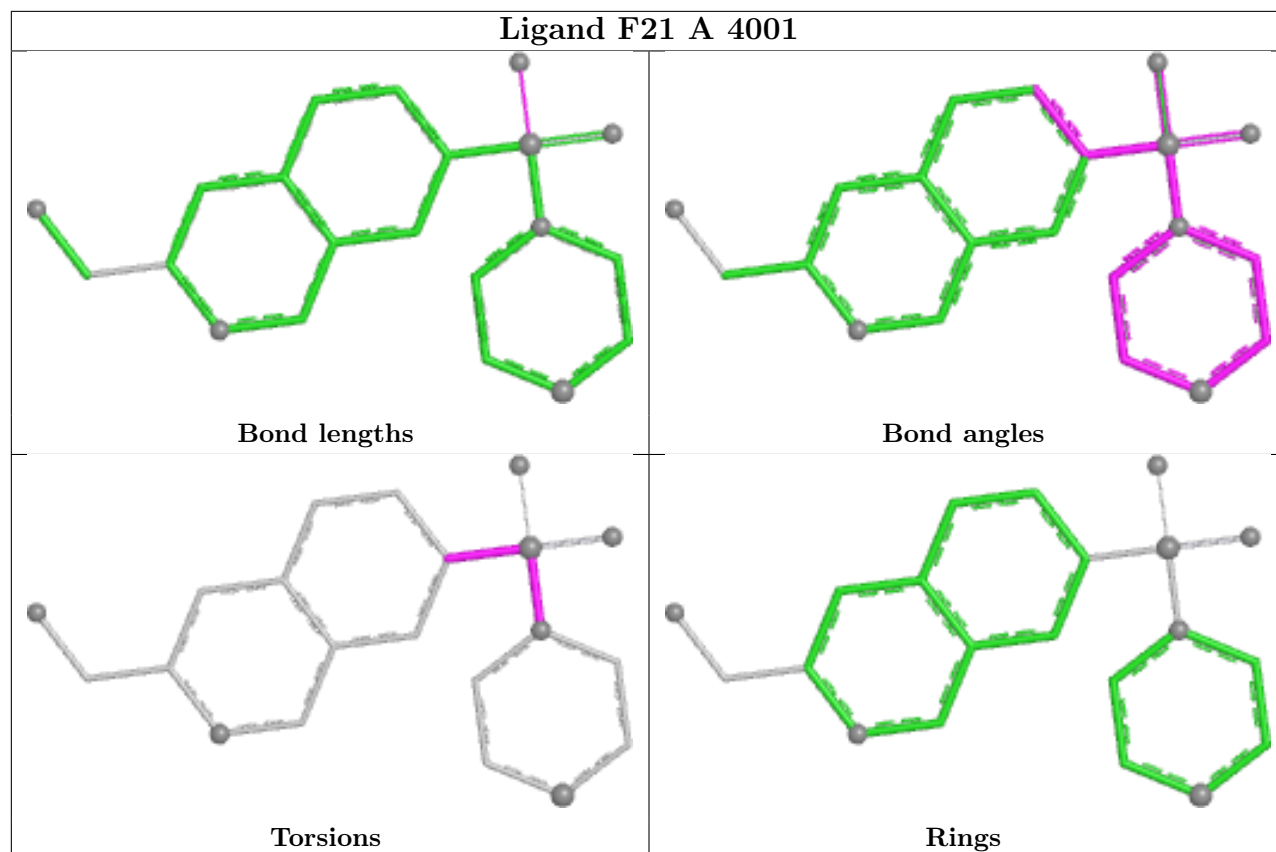
Mol	Chain	Res	Type	Atoms
2	A	4001	F21	C8-C7-S1-O2
2	A	4001	F21	C12-N1-S1-C7
3	A	3001	SAH	O4'-C1'-N9-C8
3	B	3002	SAH	O4'-C1'-N9-C8

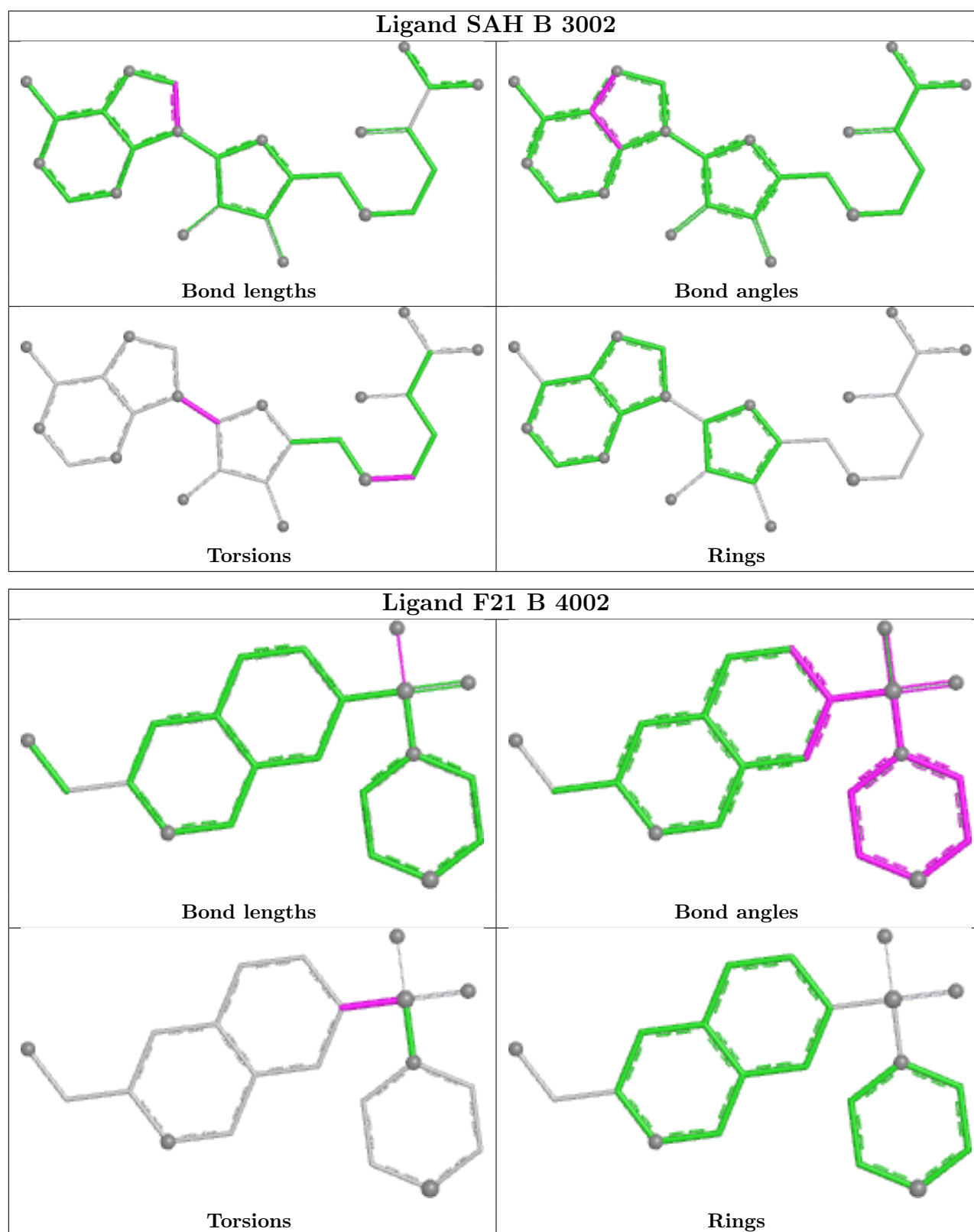
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4001	F21	2	0
3	A	3001	SAH	1	0
3	B	3002	SAH	3	0
2	B	4002	F21	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	257/289 (88%)	0.20	6 (2%)	61 51	47, 76, 100, 126	6 (2%)
1	B	268/289 (92%)	0.10	3 (1%)	78 70	47, 73, 99, 126	4 (1%)
All	All	525/578 (90%)	0.14	9 (1%)	69 60	47, 74, 100, 126	10 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	ALA	5.4
1	A	261	HIS	3.2
1	B	227	ALA	3.1
1	A	280	VAL	2.8
1	A	163	GLN	2.8
1	A	249	LYS	2.7
1	B	226	GLU	2.7
1	A	162	PRO	2.1
1	B	280	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

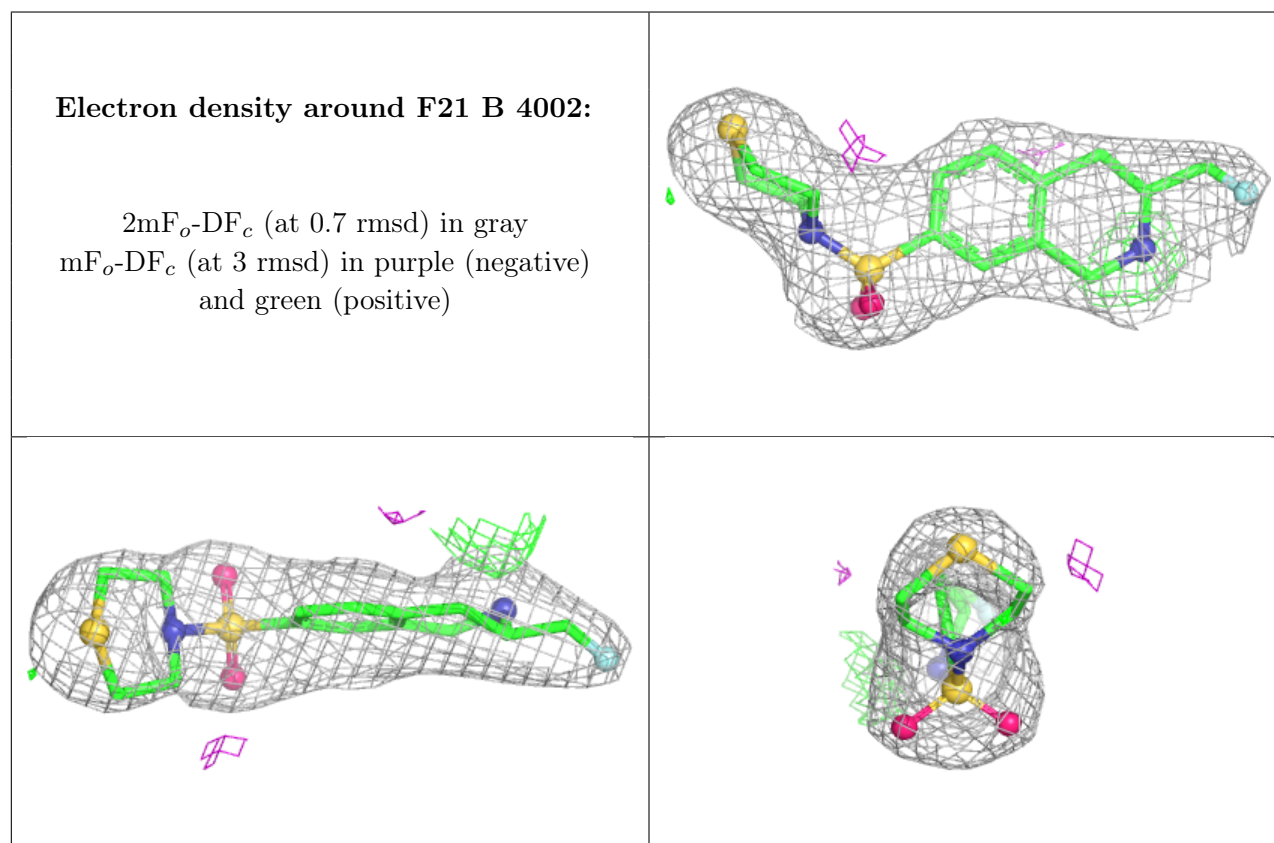
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

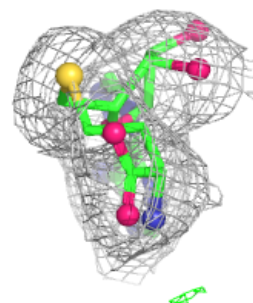
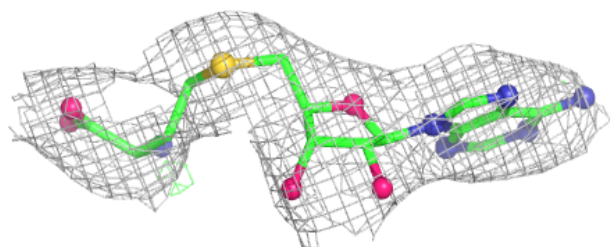
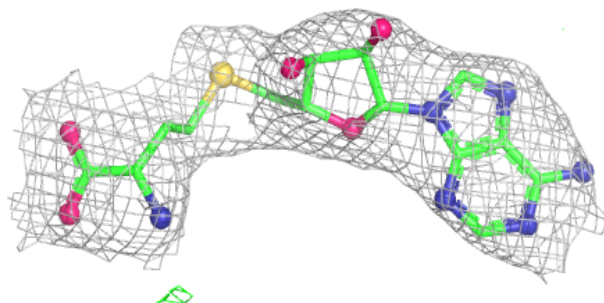
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	B	290	5/5	0.57	0.14	137,137,139,139	0
2	F21	B	4002	21/21	0.95	0.10	63,67,72,79	0
3	SAH	A	3001	26/26	0.95	0.08	49,73,75,76	0
3	SAH	B	3002	26/26	0.95	0.09	51,66,80,81	0
2	F21	A	4001	21/21	0.95	0.10	53,65,70,72	0

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.

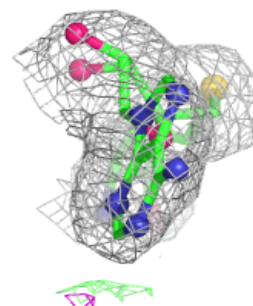
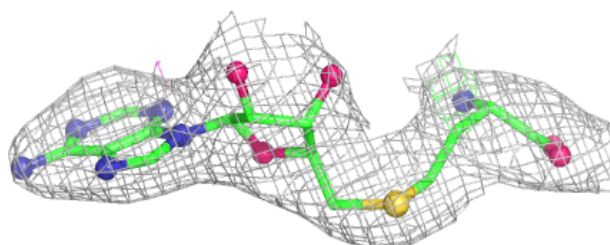
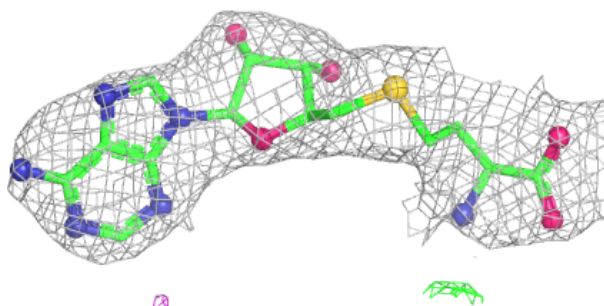


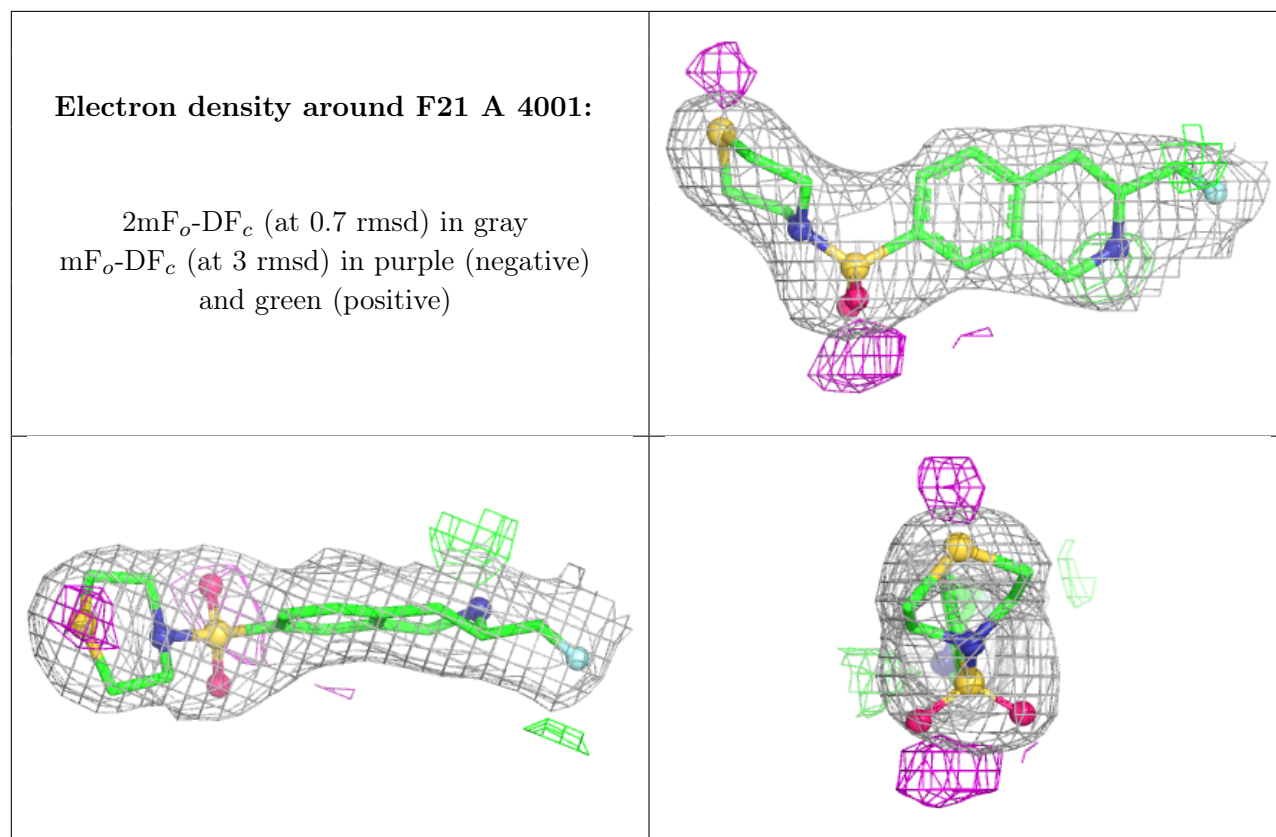
Electron density around SAH A 3001:

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

**Electron density around SAH B 3002:**

$2mF_o-DF_c$ (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.