



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:47 AM UTC

PDB ID : 1AMN / pdb_00001amn
Title : TRANSITION STATE ANALOG: ACETYLCHOLINESTERASE COM-
PLEXED WITH M-(N,N,N-TRIMETHYLAMMONIO)TRIFLUOROAC
ETOPHENONE
Authors : Harel, M.; Silman, I.; Sussman, J.L.
Deposited on : 1996-02-13
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)
Xtrriage (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

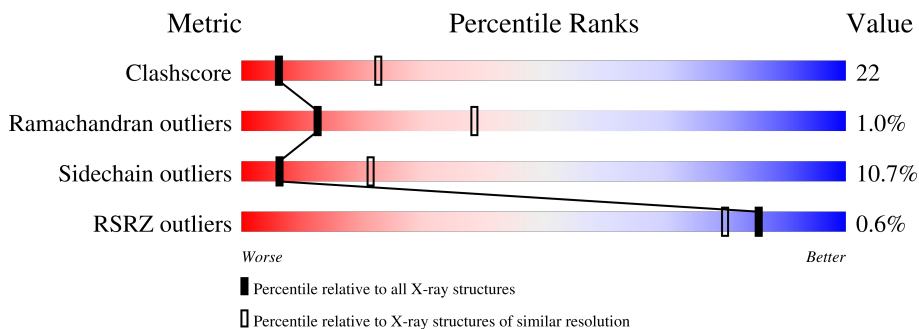
1 Overall quality at a glance

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))
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	537	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5348 atoms, of which 1078 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 ACETYLCHOLINESTERASE.

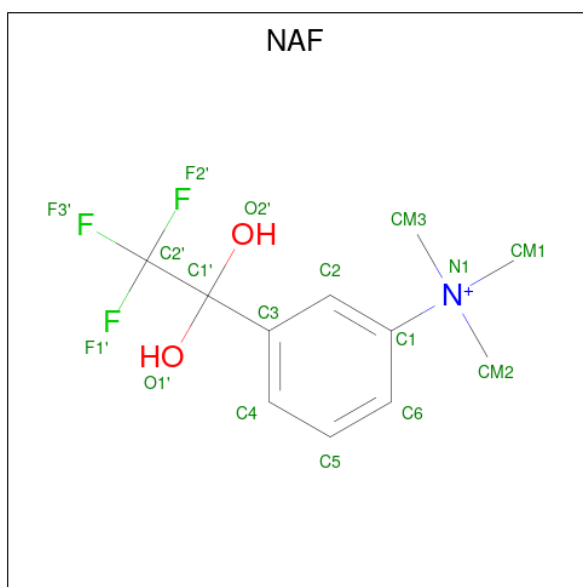
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	526	5029	2680	880	700	747	22	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is M-(N,N,N-TRIMETHYLAMMONIO)-2,2,2-TRIFLUORO-1,1-DIHYDROXY ETHYLBENZENE (CCD ID: NAF) (formula: C₁₁H₁₅F₃NO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	17	11	3	1	2	0	0

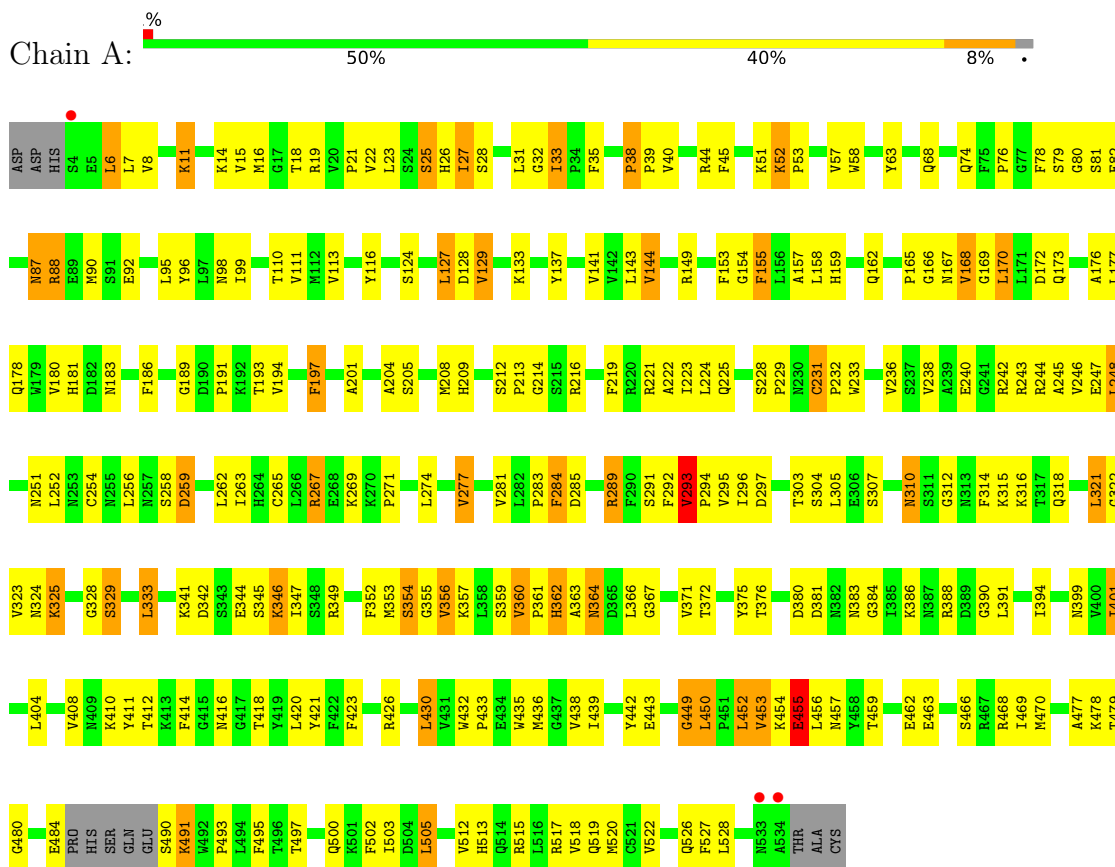
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
4	A	99	297	198	99	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ACETYLCHOLINESTERASE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.54Å 113.54Å 137.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 93.7 (8.00-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.80Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , 0.235 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtrriage
Anisotropy	0.420	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5348	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: NAF, SO4

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	0.68	0/4269	1.17	45/5795 (0.8%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	LEU	N-CA-C	8.65	123.33	109.24
1	A	231	CYS	CA-C-N	8.37	128.10	119.56
1	A	231	CYS	C-N-CA	8.37	128.10	119.56
1	A	443	GLU	N-CA-C	-8.25	103.35	113.41
1	A	133	LYS	N-CA-C	7.45	120.06	111.11
1	A	463	GLU	N-CA-C	-7.28	103.35	111.28
1	A	401	ILE	N-CA-C	7.02	117.11	110.30
1	A	439	ILE	N-CA-C	6.82	118.38	109.58
1	A	52	LYS	CA-C-N	6.72	126.75	119.90
1	A	52	LYS	C-N-CA	6.72	126.75	119.90
1	A	157	ALA	N-CA-C	6.69	121.65	107.67
1	A	346	LYS	N-CA-C	-6.49	100.68	110.28
1	A	297	ASP	N-CA-C	6.47	121.17	113.28
1	A	205	SER	N-CA-C	-6.18	104.47	111.14
1	A	527	PHE	N-CA-C	6.13	117.65	110.97
1	A	170	LEU	N-CA-C	-6.10	105.33	112.89
1	A	360	VAL	CA-C-N	6.10	125.80	119.82
1	A	360	VAL	C-N-CA	6.10	125.80	119.82
1	A	162	GLN	N-CA-C	-6.04	106.24	113.97
1	A	449	GLY	N-CA-C	5.98	124.12	114.90
1	A	82	GLU	N-CA-C	5.95	120.61	113.23
1	A	347	ILE	N-CA-C	5.91	116.44	108.17
1	A	285	ASP	N-CA-C	-5.87	100.27	109.25
1	A	165	PRO	N-CA-C	-5.82	102.45	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	TYR	N-CA-C	5.78	120.33	113.28
1	A	442	TYR	N-CA-C	5.66	119.17	112.72
1	A	479	THR	N-CA-C	5.66	121.05	114.04
1	A	364	ASN	N-CA-C	-5.59	101.69	110.36
1	A	201	ALA	N-CA-C	-5.53	105.26	112.23
1	A	457	ASN	N-CA-C	5.47	119.13	111.74
1	A	325	LYS	N-CA-C	5.46	117.04	111.14
1	A	33	ILE	N-CA-C	-5.43	103.96	108.63
1	A	480	GLY	N-CA-C	-5.39	107.76	115.64
1	A	38	PRO	CA-C-N	5.35	126.53	119.84
1	A	38	PRO	C-N-CA	5.35	126.53	119.84
1	A	6	LEU	N-CA-C	5.32	117.99	111.82
1	A	291	SER	N-CA-C	5.31	122.11	110.80
1	A	155	PHE	N-CA-C	5.29	119.50	112.30
1	A	262	LEU	N-CA-C	-5.26	105.46	111.14
1	A	222	ALA	N-CA-C	5.21	117.94	109.24
1	A	31	LEU	N-CA-C	5.20	116.99	108.52
1	A	293	VAL	N-CA-CB	-5.18	103.96	111.21
1	A	214	GLY	N-CA-C	5.17	120.13	114.40
1	A	183	ASN	N-CA-C	5.12	121.82	114.39
1	A	248	LEU	N-CA-C	-5.07	106.19	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4149	880	4000	182	0
2	A	5	0	0	0	0
3	A	17	0	13	1	0
4	A	99	198	0	4	0
All	All	4270	1078	4013	183	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 22.

All (183) 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:158:LEU:HD12	1:A:263:ILE:HD11	1.53	0.91
1:A:110:THR:HG23	1:A:193:THR:HG22	1.53	0.88
1:A:383:ASN:HB3	1:A:386:LYS:HB2	1.58	0.85
1:A:68:GLN:HG2	1:A:271:PRO:HB3	1.59	0.84
1:A:303:THR:HG22	1:A:304:SER:H	1.45	0.81
1:A:322:GLY:HA3	1:A:421:TYR:CE2	2.17	0.79
1:A:252:LEU:HD23	1:A:269:LYS:HG3	1.63	0.78
1:A:453:VAL:HG22	1:A:456:LEU:HG	1.65	0.78
1:A:322:GLY:HA3	1:A:421:TYR:CZ	2.19	0.77
1:A:11:LYS:HD2	1:A:186:PHE:HE2	1.49	0.76
1:A:204:ALA:O	1:A:208:MET:HG3	1.86	0.75
1:A:113:VAL:HA	1:A:144:VAL:HG13	1.66	0.74
1:A:324:ASN:HD22	1:A:423:PHE:HB3	1.53	0.73
1:A:345:SER:O	1:A:388:ARG:HG3	1.88	0.73
1:A:354:SER:HA	1:A:357:LYS:HE2	1.69	0.73
1:A:158:LEU:HD12	1:A:263:ILE:CD1	2.21	0.70
1:A:316:LYS:HG2	1:A:414:PHE:O	1.93	0.69
1:A:259:ASP:O	1:A:263:ILE:HG12	1.93	0.68
1:A:246:VAL:HB	1:A:256:LEU:HD23	1.75	0.68
1:A:15:VAL:HG12	1:A:58:TRP:HB3	1.74	0.67
1:A:303:THR:HG22	1:A:304:SER:N	2.08	0.67
1:A:490:SER:O	1:A:491:LYS:HB2	1.94	0.67
1:A:359:SER:O	1:A:361:PRO:HD3	1.94	0.67
1:A:213:PRO:HA	1:A:216:ARG:HE	1.60	0.66
1:A:110:THR:OG1	1:A:478:LYS:HG2	1.94	0.66
1:A:324:ASN:ND2	1:A:423:PHE:HB3	2.11	0.66
1:A:236:VAL:HG13	1:A:293:VAL:HG12	1.78	0.66
1:A:418:THR:OG1	1:A:495:PHE:HB3	1.97	0.65
1:A:355:GLY:HA3	1:A:391:LEU:HD21	1.77	0.64
1:A:149:ARG:NH2	1:A:168:VAL:HG13	2.12	0.64
1:A:380:ASP:OD1	1:A:383:ASN:HB2	1.97	0.64
1:A:495:PHE:CZ	1:A:500:GLN:HG2	2.33	0.64
1:A:359:SER:C	1:A:361:PRO:HD3	2.24	0.63
1:A:353:MET:HE3	4:A:646:HOH:O	2.00	0.62
1:A:11:LYS:HD2	1:A:186:PHE:CE2	2.34	0.62
1:A:39:PRO:HD3	1:A:95:LEU:HD12	1.82	0.62
1:A:45:PHE:O	1:A:168:VAL:HG21	2.01	0.61
1:A:111:VAL:HB	1:A:194:VAL:HG22	1.83	0.61
1:A:453:VAL:CG2	1:A:456:LEU:HG	2.32	0.60
1:A:520:MET:HE2	1:A:520:MET:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:MET:HB2	1:A:57:VAL:HG11	1.83	0.59
1:A:321:LEU:HD11	1:A:408:VAL:HG22	1.85	0.59
1:A:155:PHE:CE2	1:A:294:PRO:HG3	2.38	0.59
1:A:219:PHE:O	1:A:315:LYS:HE2	2.03	0.58
1:A:372:THR:O	1:A:376:THR:HG23	2.04	0.58
1:A:450:LEU:HD12	1:A:456:LEU:HD11	1.85	0.58
1:A:459:THR:OG1	1:A:462:GLU:HG3	2.04	0.58
1:A:87:ASN:HD22	1:A:87:ASN:C	2.12	0.57
1:A:216:ARG:HG2	1:A:315:LYS:HB2	1.85	0.57
1:A:352:PHE:O	1:A:356:VAL:HG13	2.05	0.57
1:A:310:ASN:ND2	1:A:410:LYS:HE3	2.20	0.57
1:A:453:VAL:HG23	1:A:455:GLU:HG2	1.87	0.57
1:A:242:ARG:O	1:A:245:ALA:HB3	2.05	0.57
1:A:149:ARG:NH2	1:A:168:VAL:CG1	2.68	0.56
1:A:233:TRP:O	1:A:293:VAL:HG21	2.05	0.56
1:A:236:VAL:HG13	1:A:293:VAL:CG1	2.35	0.56
1:A:6:LEU:HB3	1:A:16:MET:HE3	1.88	0.56
1:A:155:PHE:HE2	1:A:294:PRO:HG3	1.69	0.56
1:A:166:GLY:O	1:A:168:VAL:N	2.39	0.55
1:A:401:ILE:HG21	1:A:517:ARG:HG3	1.88	0.55
1:A:426:ARG:NE	4:A:633:HOH:O	2.38	0.55
1:A:197:PHE:CB	1:A:223:ILE:HB	2.36	0.55
1:A:44:ARG:HD3	1:A:92:GLU:OE2	2.06	0.55
1:A:360:VAL:CG1	1:A:363:ALA:HB2	2.36	0.55
1:A:353:MET:O	1:A:357:LYS:HG3	2.08	0.55
1:A:23:LEU:HD11	1:A:452:LEU:HD23	1.88	0.54
1:A:303:THR:CG2	1:A:304:SER:H	2.20	0.53
1:A:189:GLY:O	1:A:191:PRO:HD3	2.07	0.53
1:A:349:ARG:HD2	1:A:381:ASP:O	2.08	0.53
1:A:390:GLY:O	1:A:394:ILE:HG13	2.09	0.53
1:A:360:VAL:HG12	1:A:363:ALA:HB2	1.91	0.53
1:A:173:GLN:OE1	1:A:209:HIS:HE1	1.92	0.53
1:A:169:GLY:HA2	1:A:172:ASP:OD2	2.09	0.52
1:A:333:LEU:HD22	1:A:333:LEU:O	2.09	0.52
1:A:213:PRO:HA	1:A:216:ARG:NE	2.23	0.52
1:A:318:GLN:HG3	1:A:416:ASN:O	2.09	0.52
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.91	0.52
1:A:68:GLN:OE1	1:A:90:MET:HE3	2.10	0.51
1:A:372:THR:HG23	1:A:376:THR:HG21	1.91	0.51
1:A:312:GLY:HA2	1:A:314:PHE:CE2	2.45	0.51
1:A:110:THR:HG23	1:A:193:THR:CG2	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:HG22	1:A:512:VAL:HA	1.93	0.51
1:A:35:PHE:CZ	1:A:176:ALA:HB2	2.46	0.51
1:A:265:CYS:SG	1:A:269:LYS:HE2	2.49	0.51
1:A:254:CYS:O	1:A:256:LEU:HD12	2.11	0.51
1:A:503:ILE:HG22	1:A:512:VAL:HG22	1.92	0.51
1:A:246:VAL:O	1:A:256:LEU:HD21	2.11	0.50
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.93	0.50
1:A:33:ILE:HD12	1:A:99:ILE:HD12	1.94	0.50
1:A:8:VAL:O	1:A:14:LYS:HA	2.12	0.50
1:A:433:PRO:HB2	1:A:435:TRP:CD1	2.47	0.50
1:A:349:ARG:HH12	1:A:376:THR:HG21	1.77	0.49
1:A:325:LYS:HB3	1:A:438:VAL:HB	1.95	0.49
1:A:289:ARG:NH2	1:A:399:ASN:OD1	2.44	0.49
1:A:367:GLY:O	1:A:371:VAL:HG23	2.11	0.49
1:A:149:ARG:HH22	1:A:168:VAL:HG13	1.78	0.49
1:A:454:LYS:C	1:A:456:LEU:H	2.21	0.49
1:A:240:GLU:OE2	1:A:243:ARG:HD3	2.13	0.49
1:A:243:ARG:HG3	1:A:244:ARG:N	2.27	0.49
1:A:252:LEU:HB3	1:A:269:LYS:HE3	1.95	0.49
1:A:21:PRO:HG3	1:A:26:HIS:NE2	2.28	0.48
1:A:466:SER:O	1:A:470:MET:HG3	2.13	0.48
1:A:213:PRO:HG2	4:A:610:HOH:O	2.13	0.48
1:A:349:ARG:HD3	1:A:381:ASP:OD2	2.14	0.48
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.48	0.48
1:A:74:GLN:O	1:A:76:PRO:HD3	2.12	0.48
1:A:79:SER:O	1:A:80:GLY:C	2.55	0.48
1:A:314:PHE:CE1	1:A:411:TYR:CD2	3.01	0.48
1:A:450:LEU:HD12	1:A:456:LEU:CD1	2.43	0.48
1:A:7:LEU:C	1:A:7:LEU:HD13	2.39	0.47
1:A:149:ARG:O	1:A:154:GLY:HA3	2.15	0.47
1:A:159:HIS:HB2	1:A:238:VAL:HG13	1.95	0.47
1:A:228:SER:OG	1:A:404:LEU:HA	2.15	0.47
1:A:491:LYS:O	1:A:493:PRO:HD3	2.14	0.47
3:A:594:NAF:F1'	3:A:594:NAF:H4	2.03	0.47
1:A:137:TYR:CD1	1:A:137:TYR:C	2.93	0.47
1:A:247:GLU:HB3	1:A:281:VAL:HG12	1.96	0.47
1:A:40:VAL:HG12	1:A:92:GLU:HB2	1.97	0.47
1:A:450:LEU:O	1:A:453:VAL:HG13	2.14	0.47
1:A:208:MET:HG2	1:A:229:PRO:HB3	1.97	0.47
1:A:243:ARG:O	1:A:246:VAL:HG22	2.15	0.46
1:A:346:LYS:HB3	1:A:384:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLY:O	1:A:96:TYR:HD2	1.98	0.46
1:A:251:ASN:C	1:A:252:LEU:HD12	2.40	0.46
1:A:63:TYR:HB3	1:A:88:ARG:HD3	1.98	0.46
1:A:455:GLU:CD	1:A:455:GLU:H	2.24	0.46
1:A:324:ASN:ND2	1:A:423:PHE:HD2	2.12	0.46
1:A:366:LEU:HD12	1:A:366:LEU:HA	1.70	0.46
1:A:310:ASN:HD21	1:A:410:LYS:HE3	1.81	0.45
1:A:74:GLN:C	1:A:76:PRO:HD3	2.42	0.45
1:A:454:LYS:O	1:A:456:LEU:N	2.49	0.45
1:A:433:PRO:HG2	1:A:436:MET:SD	2.57	0.45
1:A:35:PHE:C	1:A:35:PHE:CD1	2.95	0.44
1:A:263:ILE:O	1:A:267:ARG:HB2	2.17	0.44
1:A:469:ILE:HD11	1:A:505:LEU:HD12	1.99	0.44
1:A:251:ASN:HB3	1:A:277:VAL:HG21	1.99	0.44
1:A:178:GLN:O	1:A:181:HIS:HB3	2.17	0.43
1:A:420:LEU:HD23	1:A:502:PHE:HB3	2.00	0.43
1:A:116:TYR:C	1:A:116:TYR:CD1	2.95	0.43
1:A:284:PHE:CD1	1:A:284:PHE:N	2.83	0.43
1:A:362:HIS:CD2	1:A:362:HIS:N	2.86	0.43
1:A:246:VAL:HB	1:A:256:LEU:CD2	2.46	0.43
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.77	0.43
1:A:364:ASN:OD1	1:A:364:ASN:C	2.62	0.43
1:A:33:ILE:CD1	1:A:99:ILE:HD12	2.48	0.43
1:A:44:ARG:HD2	1:A:153:PHE:HD1	1.83	0.43
1:A:197:PHE:H	1:A:197:PHE:HD1	1.66	0.43
1:A:25:SER:O	1:A:26:HIS:ND1	2.52	0.43
1:A:450:LEU:HD13	1:A:450:LEU:HA	1.73	0.43
1:A:503:ILE:CG2	1:A:512:VAL:HG22	2.48	0.43
1:A:296:ILE:CD1	1:A:305:LEU:HD13	2.49	0.42
1:A:344:GLU:O	1:A:345:SER:C	2.61	0.42
1:A:362:HIS:CD2	4:A:613:HOH:O	2.72	0.42
1:A:372:THR:HG23	1:A:376:THR:CG2	2.48	0.42
1:A:423:PHE:HD1	1:A:505:LEU:HB3	1.84	0.42
1:A:159:HIS:CB	1:A:238:VAL:HG13	2.49	0.42
1:A:221:ARG:HD2	1:A:477:ALA:O	2.20	0.42
1:A:212:SER:HA	1:A:213:PRO:HD2	1.90	0.42
1:A:231:CYS:HA	1:A:232:PRO:HD3	1.82	0.42
1:A:426:ARG:CG	1:A:430:LEU:HD12	2.50	0.42
1:A:51:LYS:HA	1:A:51:LYS:HD2	1.82	0.42
1:A:321:LEU:HD23	1:A:321:LEU:H	1.85	0.42
1:A:383:ASN:CB	1:A:386:LYS:HB2	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PHE:HE2	1:A:432:TRP:CH2	2.38	0.41
1:A:491:LYS:HD3	1:A:491:LYS:HA	1.75	0.41
1:A:52:LYS:HA	1:A:53:PRO:HD3	1.85	0.41
1:A:88:ARG:CG	1:A:88:ARG:HH11	2.33	0.41
1:A:38:PRO:HA	1:A:39:PRO:HD2	1.88	0.41
1:A:328:GLY:O	1:A:329:SER:C	2.63	0.41
1:A:124:SER:HB2	1:A:127:LEU:HD23	2.02	0.41
1:A:216:ARG:NH1	1:A:314:PHE:HA	2.36	0.41
1:A:127:LEU:O	1:A:129:VAL:N	2.54	0.41
1:A:341:LYS:HE2	1:A:342:ASP:OD1	2.21	0.41
1:A:27:ILE:HG23	1:A:28:SER:N	2.36	0.41
1:A:22:VAL:O	1:A:22:VAL:HG13	2.21	0.40
1:A:44:ARG:O	1:A:45:PHE:HB2	2.21	0.40
1:A:22:VAL:HG22	1:A:23:LEU:HG	2.04	0.40
1:A:170:LEU:HD12	1:A:170:LEU:HA	1.89	0.40
1:A:236:VAL:CG2	1:A:295:VAL:HG12	2.52	0.40
1:A:449:GLY:O	1:A:452:LEU:HB2	2.22	0.40
1:A:18:THR:HG22	1:A:19:ARG:N	2.36	0.40
1:A:248:LEU:HD22	1:A:292:PHE:CZ	2.57	0.40
1:A:98:ASN:O	1:A:144:VAL:HA	2.20	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	522/537 (97%)	473 (91%)	44 (8%)	5 (1%)	12 38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ASP

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Mol	Chain	Res	Type
1	A	167	ASN
1	A	491	LYS
1	A	329	SER
1	A	455	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	440/469 (94%)	393 (89%)	47 (11%)	6 21

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	25	SER
1	A	27	ILE
1	A	81	SER
1	A	87	ASN
1	A	88	ARG
1	A	129	VAL
1	A	141	VAL
1	A	143	LEU
1	A	144	VAL
1	A	168	VAL
1	A	177	LEU
1	A	180	VAL
1	A	197	PHE
1	A	224	LEU
1	A	225	GLN
1	A	258	SER
1	A	259	ASP
1	A	267	ARG
1	A	274	LEU
1	A	277	VAL
1	A	283	PRO

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Mol	Chain	Res	Type
1	A	284	PHE
1	A	289	ARG
1	A	293	VAL
1	A	307	SER
1	A	310	ASN
1	A	321	LEU
1	A	323	VAL
1	A	333	LEU
1	A	354	SER
1	A	356	VAL
1	A	362	HIS
1	A	412	THR
1	A	430	LEU
1	A	450	LEU
1	A	452	LEU
1	A	453	VAL
1	A	455	GLU
1	A	468	ARG
1	A	484	GLU
1	A	497	THR
1	A	505	LEU
1	A	519	GLN
1	A	522	VAL
1	A	526	GLN
1	A	528	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	74	GLN
1	A	87	ASN
1	A	131	ASN
1	A	209	HIS
1	A	225	GLN
1	A	264	HIS
1	A	310	ASN
1	A	324	ASN
1	A	398	HIS
1	A	409	ASN
1	A	416	ASN
1	A	483	ASN

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Mol	Chain	Res	Type
1	A	514	GLN
1	A	525	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](#)

2 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
3	NAF	A	594	1	16,17,17	3.14	9 (56%)	24,28,28	2.52	8 (33%)
2	SO4	A	593	-	4,4,4	1.71	1 (25%)	6,6,6	1.25	1 (16%)

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	NAF	A	594	1	-	5/21/21/21	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	594	NAF	O1'-C1'	-6.36	1.33	1.39
3	A	594	NAF	O2'-C1'	4.99	1.44	1.39
3	A	594	NAF	C1-N1	-4.93	1.39	1.50
3	A	594	NAF	C6-C1	4.49	1.49	1.39
3	A	594	NAF	C2-C3	3.26	1.44	1.39
3	A	594	NAF	C4-C3	3.09	1.44	1.39
3	A	594	NAF	F1'-C2'	3.08	1.43	1.33
3	A	594	NAF	F2'-C2'	3.04	1.43	1.33
2	A	593	SO4	O1-S	2.44	1.59	1.44
3	A	594	NAF	F3'-C2'	2.06	1.40	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	594	NAF	F2'-C2'-C1'	-5.73	107.00	111.67
3	A	594	NAF	C2'-C1'-C3	5.69	115.48	109.70
3	A	594	NAF	CM3-N1-CM2	-4.92	91.05	108.01
3	A	594	NAF	F1'-C2'-C1'	3.58	114.59	111.67
3	A	594	NAF	CM3-N1-C1	3.47	119.73	110.78
3	A	594	NAF	CM3-N1-CM1	3.10	118.70	108.01
3	A	594	NAF	CM2-N1-C1	2.40	116.97	110.78
3	A	594	NAF	CM1-N1-C1	-2.28	104.91	110.78
2	A	593	SO4	O3-S-O1	-2.15	98.31	109.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

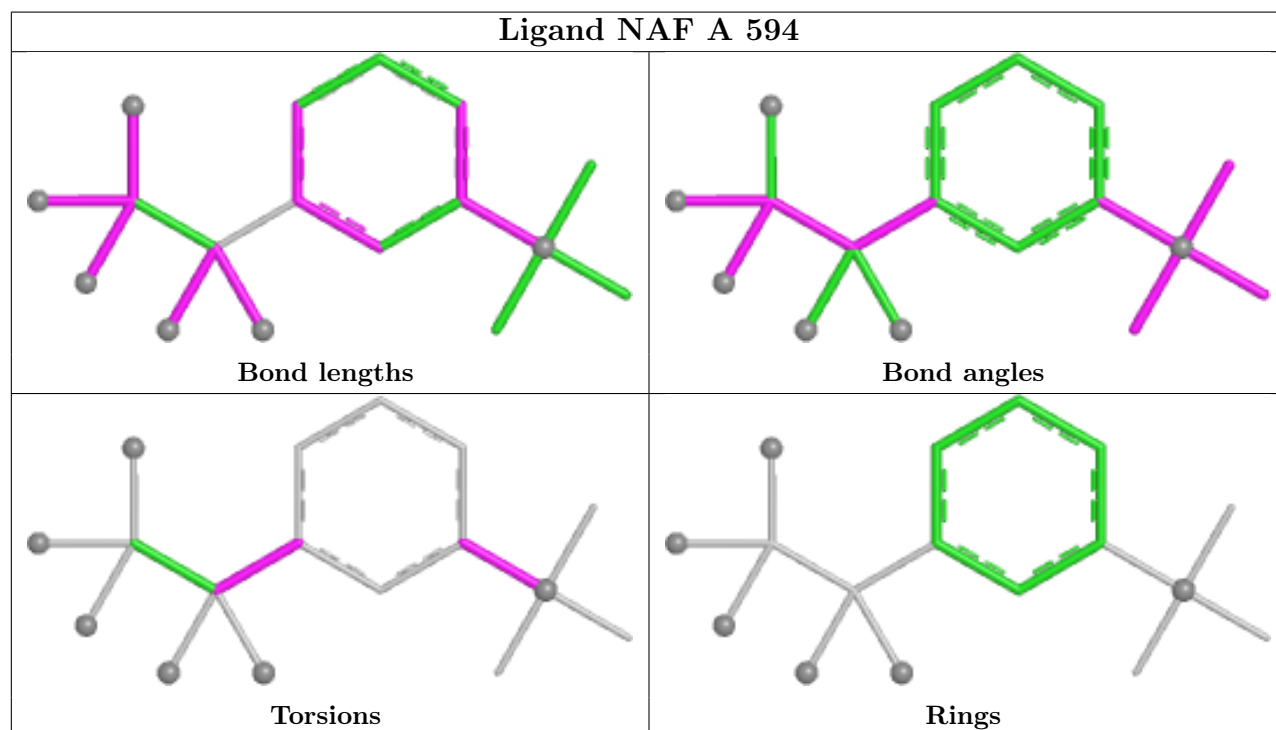
Mol	Chain	Res	Type	Atoms
3	A	594	NAF	O1'-C1'-C3-C2
3	A	594	NAF	O1'-C1'-C3-C4
3	A	594	NAF	C2'-C1'-C3-C2
3	A	594	NAF	C2'-C1'-C3-C4
3	A	594	NAF	C2-C1-N1-CM1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	594	NAF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	526/537 (97%)	-0.71	3 (0%) 85 80	4, 18, 38, 56	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	ALA	2.6
1	A	4	SER	2.2
1	A	533	ASN	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.

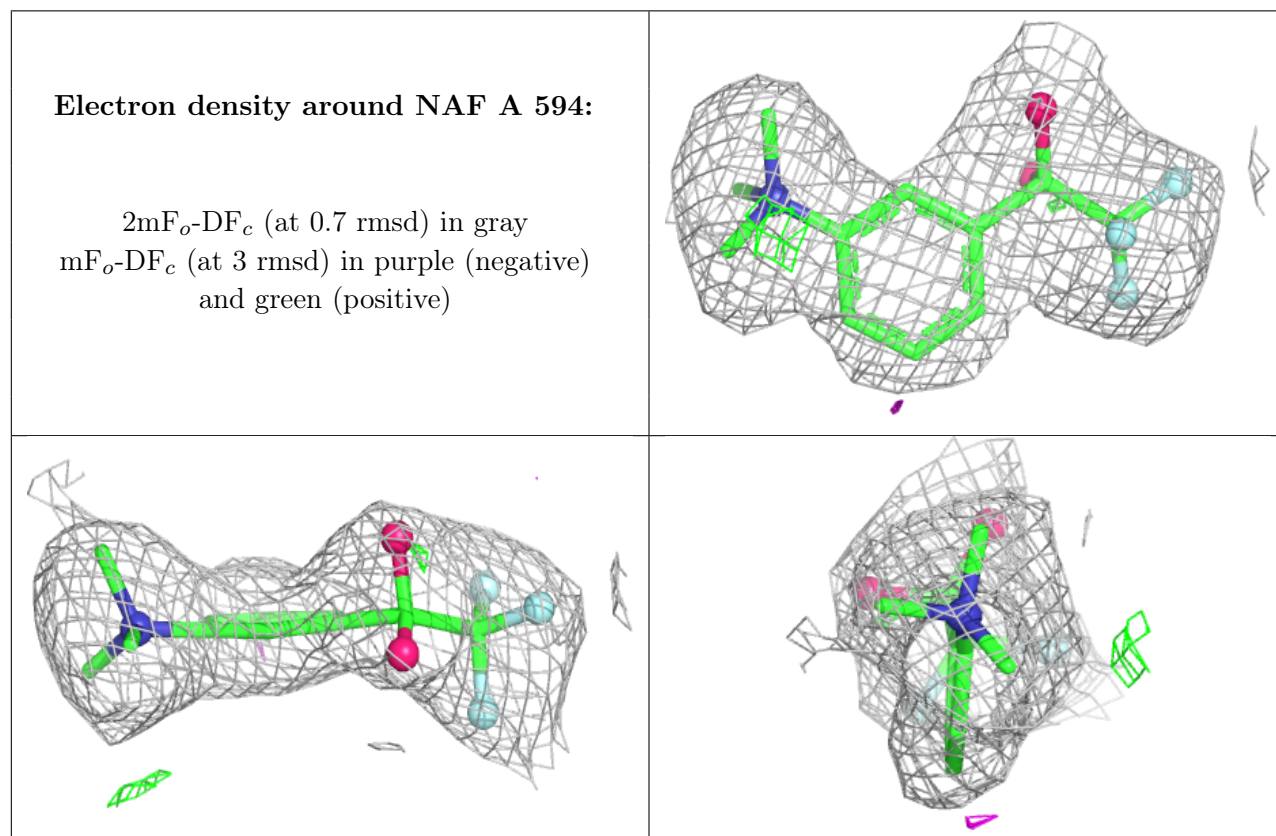
6.4 Ligands [i](#)

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	SO4	A	593	5/5	0.96	0.09	72,73,77,77	0
3	NAF	A	594	17/17	0.96	0.07	4,12,16,17	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.