



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:53 PM UTC

PDB ID : 1ZGC / pdb_00001zgc
Title : Crystal Structure of Torpedo Californica Acetylcholinesterase in Complex With an (RS)-Tacrine(10)-Hupryridone Inhibitor.
Authors : Haviv, H.; Wong, D.M.; Greenblatt, H.M.; Carlier, P.R.; Pang, Y.P.; Silman, I.; Sussman, J.L.; Israel Structural Proteomics Center (ISPC)
Deposited on : 2005-04-21
Resolution : 2.10 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

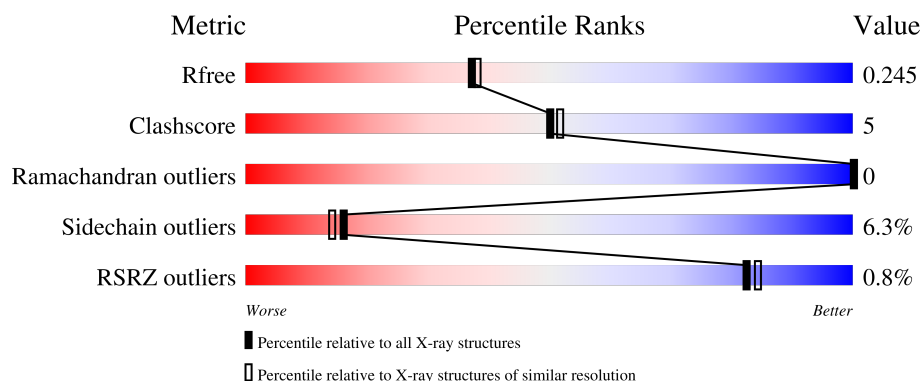
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	543	% 73% 19% • • •
1	B	543	% 72% 20% 5% • •

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
3	A2E	A	1002	-	X	-	-

2 Entry composition [i](#)

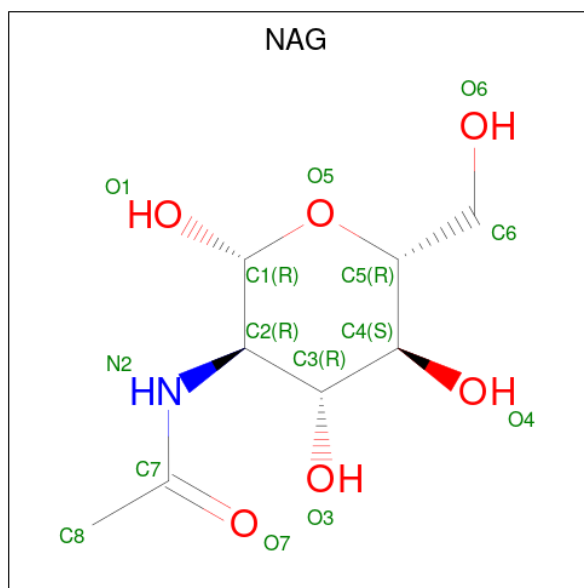
There are 4 unique types of molecules in this entry. The entry contains 8854 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	0	0
			4174	2683	702	767	22			
1	B	528	Total	C	N	O	S	0	0	0
			4195	2697	707	769	22			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



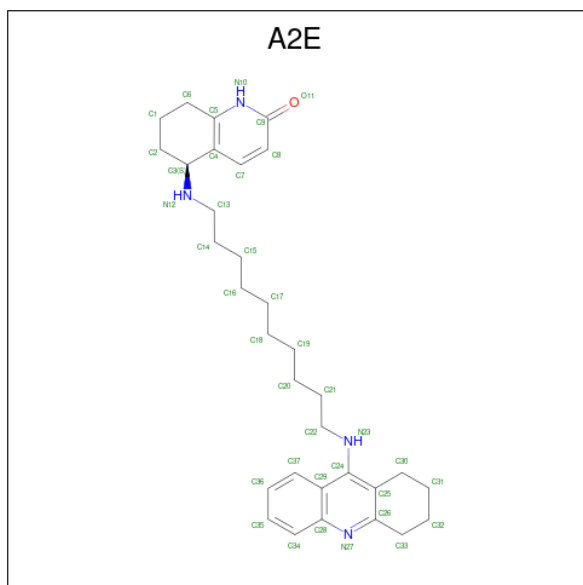
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (5S)-5-{[10-(1,2,3,4-TETRAHYDROACRIDIN-9-YLAMINO)DECYL]AMINO}-5,6,7,8-TETRAHYDROQUINOLIN-2(1H)-ONE (CCD ID: A2E) (formula: C₃₂H₄₄N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			37	32	4	1		
3	B	1	Total	C	N	O	0	0
			37	32	4	1		

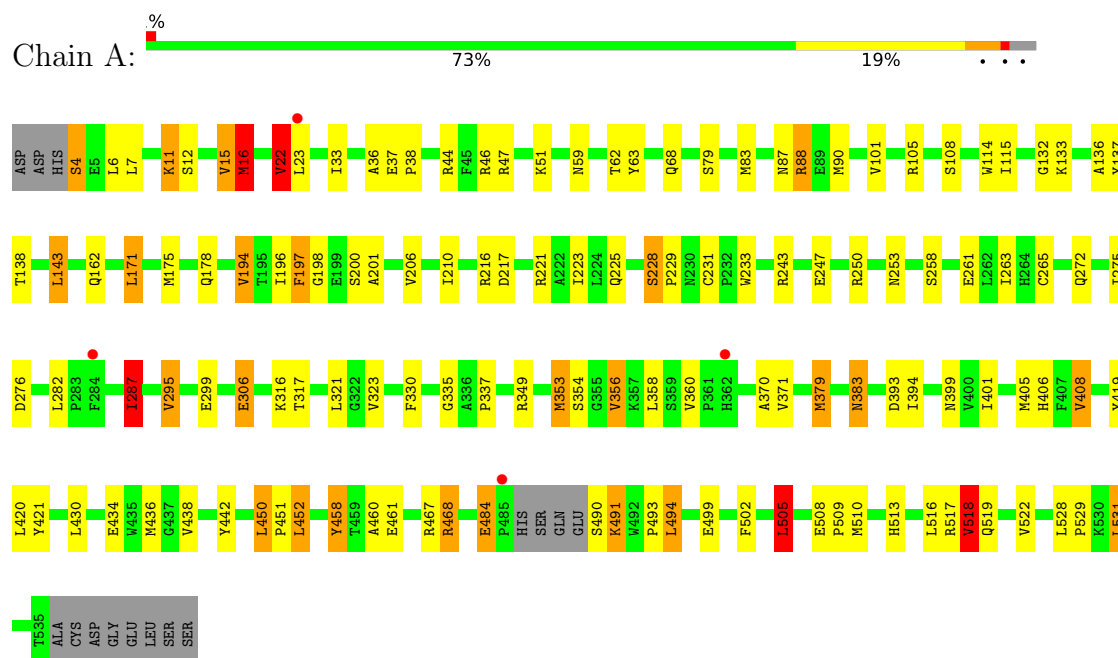
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		
4	B	168	Total	O	0	0
			168	168		

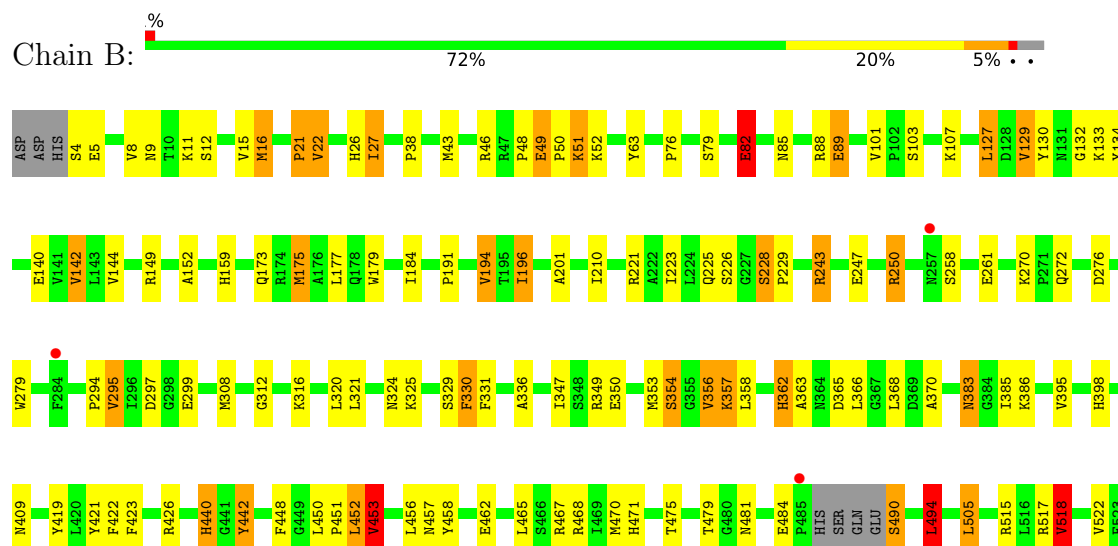
3 Residue-property plots

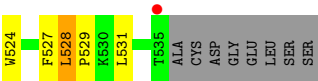
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Acetylcholinesterase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.00Å 105.54Å 150.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.10 34.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.50-2.10) 99.2 (34.50-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24, XTALVIEW	Depositor
R, R_{free}	0.196 , 0.247 (Not available) , 0.245	Depositor DCC
R_{free} test set	4157 reflections (1.77%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8854	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4117e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAG, A2E

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	1.94	66/4295 (1.5%)	1.48	39/5836 (0.7%)
1	B	1.95	77/4316 (1.8%)	1.53	43/5861 (0.7%)
All	All	1.94	143/8611 (1.7%)	1.51	82/11697 (0.7%)

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	2
1	B	0	1
All	All	0	3

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	MET	SD-CE	-24.83	1.17	1.79
1	A	175	MET	SD-CE	-19.77	1.30	1.79
1	A	16	MET	SD-CE	-15.18	1.41	1.79
1	B	51	LYS	CE-NZ	12.81	1.87	1.49
1	A	353	MET	SD-CE	12.41	2.10	1.79
1	B	16	MET	SD-CE	10.91	2.06	1.79
1	A	101	VAL	CA-CB	-9.76	1.42	1.54
1	A	379	MET	SD-CE	9.65	2.03	1.79
1	B	308	MET	SD-CE	-9.28	1.56	1.79
1	A	194	VAL	CA-CB	9.10	1.65	1.54
1	B	89	GLU	CD-OE1	8.75	1.42	1.25
1	B	395	VAL	CA-CB	-8.75	1.43	1.54
1	A	11	LYS	CE-NZ	8.24	1.74	1.49
1	A	299	GLU	CA-C	8.15	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	221	ARG	CD-NE	-8.02	1.35	1.46
1	B	453	VAL	CA-CB	7.94	1.62	1.53
1	A	356	VAL	CA-CB	7.94	1.64	1.54
1	B	329	SER	N-CA	-7.87	1.36	1.46
1	B	221	ARG	NE-CZ	-7.81	1.24	1.33
1	A	394	ILE	CA-CB	-7.74	1.45	1.54
1	B	228	SER	N-CA	-7.63	1.38	1.46
1	A	90	MET	C-O	-7.49	1.14	1.23
1	A	101	VAL	CA-C	7.32	1.59	1.53
1	B	225	GLN	C-O	-7.25	1.15	1.24
1	A	11	LYS	CD-CE	7.24	1.74	1.52
1	B	38	PRO	CA-C	7.13	1.58	1.52
1	A	519	GLN	CA-C	7.09	1.61	1.52
1	B	353	MET	SD-CE	6.98	1.97	1.79
1	A	323	VAL	CA-C	-6.97	1.44	1.52
1	B	103	SER	C-O	-6.89	1.17	1.24
1	A	136	ALA	CA-CB	-6.86	1.42	1.53
1	B	82	GLU	CB-CG	6.78	1.72	1.52
1	B	515	ARG	CA-C	-6.76	1.47	1.53
1	B	457	ASN	CB-CG	6.75	1.69	1.52
1	A	38	PRO	CA-C	6.71	1.58	1.52
1	A	46	ARG	CB-CG	6.65	1.72	1.52
1	A	370	ALA	C-O	6.60	1.31	1.24
1	B	422	PHE	C-O	6.59	1.31	1.23
1	B	152	ALA	C-O	-6.57	1.15	1.24
1	A	221	ARG	NE-CZ	-6.56	1.25	1.33
1	A	394	ILE	N-CA	6.55	1.54	1.46
1	A	225	GLN	C-O	-6.52	1.16	1.24
1	B	173	GLN	CA-C	6.49	1.61	1.52
1	A	276	ASP	C-O	-6.48	1.15	1.24
1	A	468	ARG	CA-C	6.46	1.61	1.52
1	A	323	VAL	C-O	6.44	1.30	1.23
1	A	484	GLU	CA-C	6.41	1.60	1.52
1	A	59	ASN	CA-C	6.39	1.61	1.52
1	B	194	VAL	CA-CB	6.38	1.61	1.54
1	A	393	ASP	C-O	-6.37	1.16	1.24
1	A	263	ILE	CA-CB	-6.36	1.47	1.54
1	A	59	ASN	CA-CB	6.33	1.60	1.52
1	A	261	GLU	C-O	-6.28	1.16	1.24
1	A	250	ARG	NE-CZ	6.27	1.40	1.33
1	A	171	LEU	CA-CB	6.25	1.63	1.53
1	B	142	VAL	C-O	-6.21	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	324	ASN	C-O	6.17	1.31	1.23
1	B	48	PRO	C-O	-6.16	1.16	1.23
1	B	299	GLU	CA-C	6.15	1.61	1.52
1	A	196	ILE	CA-CB	6.12	1.62	1.54
1	B	196	ILE	CA-CB	6.12	1.62	1.54
1	B	515	ARG	CZ-NH1	6.12	1.41	1.32
1	A	438	VAL	CA-C	6.09	1.59	1.53
1	A	51	LYS	N-CA	-6.09	1.38	1.46
1	A	115	ILE	CA-CB	-6.09	1.46	1.53
1	A	228	SER	N-CA	-6.09	1.39	1.46
1	B	386	LYS	CA-C	6.08	1.60	1.52
1	A	37	GLU	C-O	6.03	1.31	1.23
1	B	27	ILE	CB-CG2	6.02	1.72	1.52
1	A	275	ILE	CA-C	-5.98	1.44	1.52
1	B	354	SER	CB-OG	-5.98	1.30	1.42
1	B	8	VAL	C-O	-5.98	1.18	1.24
1	A	79	SER	C-O	-5.97	1.17	1.24
1	B	426	ARG	C-O	5.95	1.31	1.24
1	B	354	SER	CA-C	5.91	1.60	1.52
1	A	258	SER	N-CA	5.91	1.53	1.45
1	A	23	LEU	C-O	5.82	1.30	1.23
1	B	226	SER	CA-C	5.79	1.60	1.53
1	B	76	PRO	CA-C	5.77	1.59	1.52
1	B	11	LYS	CE-NZ	5.77	1.66	1.49
1	A	408	VAL	N-CA	-5.76	1.39	1.46
1	B	127	LEU	C-O	-5.75	1.17	1.23
1	A	44	ARG	C-O	5.74	1.30	1.23
1	B	16	MET	C-O	-5.73	1.17	1.24
1	B	250	ARG	NE-CZ	5.71	1.39	1.33
1	A	11	LYS	CB-CG	5.71	1.69	1.52
1	A	516	LEU	C-O	5.69	1.30	1.24
1	A	371	VAL	CA-CB	5.68	1.61	1.54
1	B	79	SER	C-O	-5.68	1.17	1.24
1	B	179	TRP	CA-C	5.67	1.60	1.52
1	B	201	ALA	C-O	-5.65	1.16	1.24
1	A	460	ALA	CA-CB	5.64	1.62	1.53
1	B	276	ASP	C-O	-5.63	1.17	1.24
1	B	243	ARG	C-O	5.60	1.30	1.24
1	A	458	TYR	CA-C	5.57	1.60	1.52
1	B	442	TYR	N-CA	5.57	1.53	1.46
1	B	321	LEU	C-O	-5.56	1.17	1.23
1	A	11	LYS	CG-CD	5.55	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	505	LEU	N-CA	-5.53	1.40	1.46
1	A	317	THR	C-O	-5.52	1.20	1.24
1	A	105	ARG	CA-C	5.51	1.59	1.53
1	A	354	SER	CA-C	5.50	1.60	1.52
1	A	36	ALA	CA-CB	-5.50	1.43	1.53
1	B	21	PRO	CA-CB	5.47	1.61	1.53
1	B	465	LEU	C-O	-5.45	1.17	1.24
1	B	51	LYS	CB-CG	5.45	1.68	1.52
1	B	9	ASN	CB-CG	5.45	1.65	1.52
1	A	63	TYR	CA-C	5.43	1.59	1.53
1	B	398	HIS	CA-C	5.43	1.59	1.52
1	B	43	MET	CG-SD	-5.42	1.67	1.80
1	B	481	ASN	CA-C	5.42	1.59	1.52
1	B	101	VAL	CA-CB	-5.41	1.47	1.54
1	B	370	ALA	C-O	5.40	1.30	1.24
1	B	321	LEU	N-CA	-5.34	1.39	1.46
1	A	33	ILE	CA-CB	-5.33	1.47	1.54
1	B	350	GLU	CA-C	5.33	1.59	1.52
1	B	448	PHE	CD1-CE1	5.32	1.54	1.38
1	A	216	ARG	C-O	5.31	1.30	1.24
1	B	409	ASN	CB-CG	5.30	1.65	1.52
1	B	479	THR	CA-CB	5.28	1.62	1.54
1	A	87	ASN	C-O	-5.25	1.16	1.24
1	B	63	TYR	CD2-CE2	5.24	1.54	1.38
1	B	528	LEU	N-CA	-5.24	1.41	1.46
1	B	457	ASN	CA-CB	5.23	1.62	1.53
1	A	231	CYS	CA-CB	-5.21	1.45	1.53
1	A	201	ALA	C-O	-5.21	1.17	1.24
1	B	357	LYS	CD-CE	5.20	1.68	1.52
1	B	132	GLY	C-O	-5.19	1.17	1.23
1	B	336	ALA	CA-C	-5.19	1.46	1.52
1	B	27	ILE	C-O	-5.17	1.18	1.24
1	B	149	ARG	CA-C	-5.17	1.46	1.52
1	A	137	TYR	C-O	-5.17	1.18	1.24
1	B	330	PHE	CA-C	5.14	1.59	1.52
1	B	11	LYS	CD-CE	5.14	1.67	1.52
1	A	206	VAL	N-CA	-5.11	1.40	1.46
1	B	191	PRO	CG-CD	5.08	1.68	1.50
1	B	426	ARG	CZ-NH2	5.08	1.40	1.33
1	A	438	VAL	CB-CG2	5.07	1.69	1.52
1	B	363	ALA	C-O	-5.06	1.17	1.23
1	B	423	PHE	CA-C	5.05	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	GLN	N-CA	-5.05	1.40	1.46
1	B	279	TRP	C-O	-5.03	1.17	1.24
1	B	470	MET	C-O	5.03	1.30	1.24

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ARG	NE-CZ-NH2	-12.90	107.59	119.20
1	A	518	VAL	CB-CA-C	-12.42	95.38	112.14
1	B	518	VAL	CB-CA-C	-11.27	96.93	112.14
1	A	221	ARG	NE-CZ-NH2	-9.85	110.34	119.20
1	B	221	ARG	NE-CZ-NH1	9.62	131.12	121.50
1	B	22	VAL	CB-CA-C	-9.34	95.97	111.29
1	B	349	ARG	NE-CZ-NH2	-9.10	111.01	119.20
1	B	221	ARG	CD-NE-CZ	8.00	135.59	124.40
1	A	88	ARG	CG-CD-NE	-7.74	94.97	112.00
1	A	405	MET	N-CA-C	-7.49	103.13	111.82
1	A	22	VAL	CB-CA-C	-7.29	99.34	111.29
1	B	354	SER	CB-CA-C	7.13	124.92	110.38
1	B	50	PRO	CA-C-O	-7.04	113.39	121.56
1	A	337	PRO	CA-C-O	-7.02	113.03	121.03
1	A	518	VAL	N-CA-CB	6.94	119.98	110.54
1	A	287	ILE	CA-CB-CG2	6.92	122.26	110.50
1	A	11	LYS	CD-CE-NZ	6.81	133.70	111.90
1	A	243	ARG	CG-CD-NE	-6.80	97.03	112.00
1	A	517	ARG	CG-CD-NE	-6.77	97.11	112.00
1	A	354	SER	CB-CA-C	6.76	123.65	110.67
1	A	221	ARG	NE-CZ-NH1	6.73	128.23	121.50
1	A	295	VAL	CB-CA-C	-6.71	100.61	110.81
1	B	51	LYS	CG-CD-CE	6.61	126.50	111.30
1	B	517	ARG	CA-CB-CG	-6.57	100.97	114.10
1	B	177	LEU	N-CA-C	6.45	118.31	111.28
1	A	349	ARG	NE-CZ-NH2	-6.43	113.41	119.20
1	B	515	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	B	82	GLU	CB-CG-CD	-6.41	101.70	112.60
1	A	491	LYS	N-CA-C	6.30	118.79	108.52
1	A	138	THR	N-CA-C	-6.29	103.96	111.69
1	B	462	GLU	N-CA-C	-6.12	104.16	111.69
1	A	210	ILE	N-CA-C	-6.10	104.56	110.72
1	B	129	VAL	CB-CA-C	-6.03	98.08	111.77
1	A	436	MET	N-CA-C	-5.94	105.86	113.23
1	B	51	LYS	N-CA-C	-5.89	101.56	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	MET	CG-SD-CE	5.86	113.80	100.90
1	B	524	TRP	N-CA-C	5.86	117.74	111.36
1	B	295	VAL	CB-CA-C	-5.80	101.99	110.81
1	A	15	VAL	N-CA-CB	-5.76	102.01	111.45
1	A	162	GLN	N-CA-C	-5.71	106.32	113.28
1	B	22	VAL	CG1-CB-CG2	5.69	123.33	110.80
1	B	356	VAL	N-CA-C	5.69	116.43	110.62
1	B	82	GLU	N-CA-C	5.68	119.31	112.38
1	B	210	ILE	N-CA-C	-5.64	104.86	110.62
1	A	253	ASN	CB-CA-C	-5.61	103.76	111.73
1	B	426	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	B	46	ARG	CB-CA-C	-5.55	100.11	109.83
1	A	11	LYS	CB-CG-CD	5.55	124.07	111.30
1	A	62	THR	N-CA-C	5.53	117.59	109.24
1	B	173	GLN	N-CA-C	-5.48	105.21	111.07
1	A	287	ILE	CB-CA-C	5.47	118.93	110.50
1	B	88	ARG	CG-CD-NE	-5.45	100.02	112.00
1	B	325	LYS	N-CA-C	5.44	117.21	111.28
1	B	347	ILE	N-CA-CB	-5.44	104.61	111.46
1	A	200	SER	CB-CA-C	-5.43	109.84	117.23
1	A	356	VAL	N-CA-CB	5.41	117.90	110.54
1	A	401	ILE	N-CA-C	5.37	115.51	110.30
1	B	4	SER	CA-C-N	5.36	128.20	120.38
1	B	4	SER	C-N-CA	5.36	128.20	120.38
1	B	144	VAL	CB-CA-C	-5.34	102.69	110.81
1	B	453	VAL	CA-CB-CG2	5.33	119.45	110.40
1	A	493	PRO	CA-C-N	5.32	128.40	120.95
1	A	493	PRO	C-N-CA	5.32	128.40	120.95
1	A	178	GLN	N-CA-C	-5.32	105.48	111.28
1	A	221	ARG	CD-NE-CZ	5.32	131.84	124.40
1	A	461	GLU	N-CA-C	-5.30	105.55	112.23
1	B	518	VAL	N-CA-CB	5.30	117.75	110.54
1	A	217	ASP	N-CA-C	-5.28	106.61	113.16
1	B	349	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	B	494	LEU	CA-CB-CG	5.27	134.74	116.30
1	A	399	ASN	N-CA-C	5.27	119.80	112.90
1	B	329	SER	CA-C-N	-5.26	112.70	120.28
1	B	329	SER	C-N-CA	-5.26	112.70	120.28
1	B	5	GLU	N-CA-CB	-5.23	101.87	110.14
1	A	531	LEU	CB-CG-CD1	5.21	126.33	110.70
1	B	52	LYS	N-CA-CB	5.19	117.05	110.04
1	B	107	LYS	CA-C-N	-5.13	111.75	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	LYS	C-N-CA	-5.13	111.75	121.54
1	A	83	MET	CG-SD-CE	5.12	112.16	100.90
1	A	306	GLU	N-CA-C	-5.09	105.81	111.36
1	B	52	LYS	CA-CB-CG	5.04	124.19	114.10
1	A	194	VAL	N-CA-CB	5.01	118.06	111.25

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	484	GLU	Peptide
1	A	490	SER	Peptide
1	B	440	HIS	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	4174	0	3990	38	0
1	B	4195	0	4035	50	0
2	A	42	0	39	0	0
2	B	28	0	26	0	0
3	A	37	0	44	2	0
3	B	37	0	44	1	0
4	A	173	0	0	5	0
4	B	168	0	0	5	0
All	All	8854	0	8178	89	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 5.

All (89) 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:11:LYS:CE	1:A:11:LYS:NZ	1.74	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:MET:CE	1:B:16:MET:SD	2.06	1.43
1:A:379:MET:SD	1:A:379:MET:CE	2.03	1.43
1:A:353:MET:SD	1:A:353:MET:CE	2.10	1.38
1:B:51:LYS:CE	1:B:51:LYS:NZ	1.87	1.34
1:B:175:MET:CE	1:B:175:MET:SD	1.17	1.27
1:B:175:MET:SD	1:B:175:MET:HE2	1.75	1.17
1:B:175:MET:SD	1:B:175:MET:HE3	1.75	1.16
1:B:175:MET:SD	1:B:175:MET:HE1	1.75	1.16
1:B:175:MET:CE	1:B:175:MET:CG	2.38	1.02
1:B:362:HIS:H	1:B:362:HIS:CD2	2.02	0.77
1:B:82:GLU:HG3	1:B:85:ASN:HD22	1.49	0.76
1:A:468:ARG:HD3	4:A:1583:HOH:O	1.86	0.74
1:B:26:HIS:O	1:B:27:ILE:HG23	1.92	0.70
1:B:471:HIS:CD2	1:B:475:THR:OG1	2.45	0.68
1:B:366:LEU:CD2	1:B:531:LEU:HD11	2.23	0.68
1:A:7:LEU:HB2	1:A:16:MET:HE1	1.76	0.67
1:A:419:TYR:CZ	1:A:494:LEU:HD13	2.31	0.66
1:B:362:HIS:H	1:B:362:HIS:HD2	1.42	0.64
1:B:26:HIS:O	1:B:27:ILE:CG2	2.46	0.63
1:A:379:MET:CE	1:A:379:MET:CG	2.78	0.62
1:A:306:GLU:OE1	1:A:406:HIS:HE1	1.83	0.61
1:A:383:ASN:C	1:A:383:ASN:HD22	2.09	0.60
1:B:383:ASN:C	1:B:383:ASN:HD22	2.09	0.60
1:B:366:LEU:HD23	1:B:531:LEU:HD11	1.85	0.59
1:B:421:TYR:HB2	1:B:505:LEU:HD22	1.84	0.59
1:B:453:VAL:HG22	1:B:456:LEU:HG	1.84	0.59
1:A:7:LEU:HB2	1:A:16:MET:CE	2.33	0.58
1:A:265:CYS:HB2	4:A:1610:HOH:O	2.05	0.57
1:A:22:VAL:HG13	1:A:133:LYS:HG3	1.87	0.56
1:A:452:LEU:HD13	1:A:467:ARG:NH2	2.21	0.55
1:A:228:SER:HB2	1:A:229:PRO:HD2	1.89	0.54
1:B:452:LEU:HD13	1:B:467:ARG:NH2	2.24	0.53
1:B:442:TYR:HE1	3:B:1001:A2E:H331	1.74	0.53
1:A:518:VAL:O	1:A:522:VAL:HG23	2.09	0.53
1:A:421:TYR:HB2	1:A:505:LEU:HD22	1.91	0.52
1:B:127:LEU:HD12	1:B:130:TYR:CE2	2.44	0.52
1:A:272:GLN:HG3	4:A:1611:HOH:O	2.11	0.51
1:B:228:SER:HB2	1:B:229:PRO:HD2	1.91	0.51
1:B:452:LEU:HD13	1:B:467:ARG:CZ	2.41	0.51
1:B:159:HIS:HE1	1:B:297:ASP:O	1.94	0.51
1:B:272:GLN:NE2	4:B:4174:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:PRO:HA	1:B:26:HIS:HD2	1.77	0.50
1:A:47:ARG:HG2	1:A:171:LEU:CD1	2.42	0.49
1:B:272:GLN:HG3	4:B:4271:HOH:O	2.10	0.49
1:B:490:SER:HB2	4:B:4296:HOH:O	2.11	0.49
1:A:272:GLN:NE2	4:A:1527:HOH:O	2.45	0.49
1:B:51:LYS:NZ	1:B:51:LYS:CD	2.74	0.49
1:B:142:VAL:HG11	1:B:184:ILE:HD11	1.94	0.49
1:B:518:VAL:O	1:B:522:VAL:HG23	2.14	0.48
1:A:132:GLY:HA3	1:A:143:LEU:HD22	1.96	0.48
1:B:471:HIS:HD2	1:B:475:THR:OG1	1.95	0.48
1:B:451:PRO:HA	1:B:458:TYR:CD1	2.49	0.47
3:A:1002:A2E:H21	3:A:1002:A2E:H132	1.63	0.47
1:B:468:ARG:HD3	4:B:4192:HOH:O	2.15	0.46
1:A:247:GLU:OE2	4:A:1615:HOH:O	2.20	0.46
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.51	0.46
1:A:450:LEU:N	1:A:451:PRO:CD	2.79	0.46
1:B:383:ASN:HD21	1:B:385:ILE:HB	1.81	0.46
1:A:114:TRP:CZ3	1:A:198:GLY:HA2	2.51	0.45
1:B:419:TYR:CZ	1:B:494:LEU:HD13	2.51	0.45
1:A:442:TYR:HE1	3:A:1002:A2E:H331	1.82	0.45
1:A:321:LEU:O	1:A:420:LEU:HA	2.17	0.45
1:B:133:LYS:HE2	1:B:134:TYR:CZ	2.52	0.45
1:B:331:PHE:CE1	1:B:440:HIS:HD2	2.34	0.44
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.99	0.44
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.52	0.44
1:B:223:ILE:HA	1:B:320:LEU:O	2.17	0.44
1:B:528:LEU:N	1:B:529:PRO:CD	2.81	0.44
1:B:527:PHE:O	1:B:528:LEU:C	2.58	0.44
1:B:383:ASN:C	1:B:383:ASN:ND2	2.75	0.43
1:A:430:LEU:HD11	1:A:442:TYR:CD2	2.53	0.43
1:B:331:PHE:HE1	1:B:440:HIS:HD2	1.66	0.43
1:B:468:ARG:HD2	4:B:4315:HOH:O	2.18	0.43
1:A:47:ARG:HG2	1:A:171:LEU:HD13	2.00	0.43
1:B:258:SER:OG	1:B:261:GLU:HG3	2.20	0.42
1:A:6:LEU:O	1:A:16:MET:HE2	2.19	0.42
1:B:247:GLU:OE2	1:B:250:ARG:NH2	2.46	0.42
1:B:357:LYS:HD3	1:B:368:LEU:HD11	2.01	0.42
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.87	0.41
1:B:49:GLU:C	1:B:175:MET:HE1	2.45	0.41
1:A:233:TRP:CD1	1:A:233:TRP:H	2.39	0.41
1:B:312:GLY:O	1:B:316:LYS:NZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:HB3	1:A:7:LEU:HB3	2.01	0.41
1:A:287:ILE:HD11	1:A:335:GLY:C	2.46	0.41
1:A:508:GLU:HB3	1:A:509:PRO:HD2	2.03	0.41
1:A:197:PHE:HB3	1:A:223:ILE:HB	2.02	0.40
1:B:196:ILE:HD13	1:B:196:ILE:HG21	1.91	0.40
1:A:197:PHE:CB	1:A:223:ILE:HB	2.51	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	524/543 (96%)	507 (97%)	17 (3%)	0	100	100
1	B	524/543 (96%)	503 (96%)	21 (4%)	0	100	100
All	All	1048/1086 (96%)	1010 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	449/474 (95%)	420 (94%)	29 (6%)	15	13
1	B	453/474 (96%)	425 (94%)	28 (6%)	16	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	902/948 (95%)	845 (94%)	57 (6%)	16	14

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	12	SER
1	A	15	VAL
1	A	16	MET
1	A	22	VAL
1	A	88	ARG
1	A	108	SER
1	A	143	LEU
1	A	194	VAL
1	A	197	PHE
1	A	287	ILE
1	A	295	VAL
1	A	316	LYS
1	A	330	PHE
1	A	356	VAL
1	A	358	LEU
1	A	360	VAL
1	A	383	ASN
1	A	408	VAL
1	A	434	GLU
1	A	450	LEU
1	A	452	LEU
1	A	491	LYS
1	A	494	LEU
1	A	499	GLU
1	A	505	LEU
1	A	510	MET
1	A	518	VAL
1	A	531	LEU
1	B	12	SER
1	B	15	VAL
1	B	22	VAL
1	B	49	GLU
1	B	82	GLU
1	B	89	GLU
1	B	129	VAL
1	B	140	GLU

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Mol	Chain	Res	Type
1	B	194	VAL
1	B	243	ARG
1	B	270	LYS
1	B	294	PRO
1	B	295	VAL
1	B	330	PHE
1	B	354	SER
1	B	356	VAL
1	B	358	LEU
1	B	362	HIS
1	B	365	ASP
1	B	383	ASN
1	B	450	LEU
1	B	452	LEU
1	B	453	VAL
1	B	484	GLU
1	B	490	SER
1	B	494	LEU
1	B	505	LEU
1	B	518	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	257	ASN
1	A	272	GLN
1	A	383	ASN
1	A	406	HIS
1	B	42	ASN
1	B	65	ASN
1	B	68	GLN
1	B	159	HIS
1	B	272	GLN
1	B	362	HIS
1	B	374	GLN
1	B	383	ASN
1	B	409	ASN
1	B	457	ASN
1	B	471	HIS
1	B	526	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	NAG	A	1416	1	14,14,15	1.20	3 (21%)	17,19,21	1.78	4 (23%)
3	A2E	B	1001	-	41,41,41	3.85	23 (56%)	47,54,54	2.84	16 (34%)
2	NAG	A	1059	1	14,14,15	1.87	4 (28%)	17,19,21	3.68	7 (41%)
2	NAG	A	1457	1	14,14,15	1.13	0	17,19,21	2.86	8 (47%)
2	NAG	B	1592	1	14,14,15	2.22	7 (50%)	17,19,21	3.18	12 (70%)
2	NAG	B	4162	1	14,14,15	1.22	1 (7%)	17,19,21	2.41	6 (35%)
3	A2E	A	1002	-	41,41,41	3.80	25 (60%)	47,54,54	2.45	19 (40%)

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
2	NAG	A	1416	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2E	B	1001	-	-	13/15/32/32	0/5/5/5
2	NAG	A	1059	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1457	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1592	1	-	2/6/23/26	0/1/1/1
2	NAG	B	4162	1	-	2/6/23/26	0/1/1/1
3	A2E	A	1002	-	-	12/15/32/32	0/5/5/5

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	A2E	C35-C34	9.19	1.55	1.36
3	A	1002	A2E	C33-C26	-8.75	1.37	1.50
3	A	1002	A2E	C24-C25	8.31	1.52	1.39
3	B	1001	A2E	C36-C37	8.13	1.53	1.36
3	B	1001	A2E	C33-C26	-7.38	1.39	1.50
3	B	1001	A2E	C34-C28	7.23	1.53	1.41
3	B	1001	A2E	C5-C4	7.12	1.47	1.37
3	B	1001	A2E	C35-C36	6.93	1.53	1.38
3	A	1002	A2E	C5-C4	6.92	1.46	1.37
3	B	1001	A2E	C30-C25	-6.85	1.41	1.51
3	A	1002	A2E	C30-C25	-6.80	1.41	1.51
3	A	1002	A2E	C35-C34	6.76	1.50	1.36
3	A	1002	A2E	C36-C37	5.84	1.48	1.36
3	B	1001	A2E	C24-C25	5.48	1.48	1.39
3	A	1002	A2E	C35-C36	5.23	1.49	1.38
3	B	1001	A2E	C24-C29	4.96	1.51	1.43
3	A	1002	A2E	C26-N27	4.88	1.38	1.32
3	A	1002	A2E	C29-C28	4.77	1.50	1.42
3	A	1002	A2E	C37-C29	4.56	1.51	1.42
3	A	1002	A2E	C24-C29	4.36	1.50	1.43
3	A	1002	A2E	C31-C30	-4.36	1.36	1.51
3	B	1001	A2E	C29-C28	4.20	1.49	1.42
3	A	1002	A2E	O11-C9	4.10	1.32	1.24
3	A	1002	A2E	C13-N12	3.93	1.55	1.47
3	A	1002	A2E	C2-C3	3.81	1.59	1.53
3	B	1001	A2E	C37-C29	3.74	1.49	1.42
3	A	1002	A2E	C31-C32	-3.62	1.38	1.51
2	B	1592	NAG	C4-C5	3.61	1.60	1.53
3	B	1001	A2E	C31-C30	-3.59	1.38	1.51
3	B	1001	A2E	C6-C5	3.56	1.55	1.49
3	A	1002	A2E	C34-C28	3.54	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1059	NAG	O5-C1	3.54	1.49	1.43
2	B	1592	NAG	C1-C2	3.48	1.57	1.52
3	B	1001	A2E	O11-C9	3.42	1.31	1.24
2	A	1059	NAG	C1-C2	3.27	1.56	1.52
2	A	1059	NAG	O5-C5	3.23	1.49	1.43
3	B	1001	A2E	C32-C33	-3.17	1.40	1.51
3	B	1001	A2E	C28-N27	-3.15	1.32	1.37
2	B	1592	NAG	C3-C2	3.07	1.58	1.52
3	A	1002	A2E	C32-C33	-3.04	1.40	1.51
3	A	1002	A2E	C3-C4	3.04	1.55	1.51
3	A	1002	A2E	C7-C4	-3.01	1.38	1.45
2	B	4162	NAG	O5-C5	2.96	1.49	1.43
3	B	1001	A2E	C2-C3	2.88	1.58	1.53
3	B	1001	A2E	C13-N12	2.87	1.53	1.47
3	B	1001	A2E	C31-C32	-2.86	1.41	1.51
2	B	1592	NAG	O5-C5	2.75	1.48	1.43
3	B	1001	A2E	C3-C4	2.74	1.54	1.51
2	B	1592	NAG	C6-C5	2.70	1.60	1.51
3	A	1002	A2E	C3-N12	2.67	1.52	1.46
3	B	1001	A2E	C25-C26	2.57	1.44	1.40
3	B	1001	A2E	C3-N12	2.48	1.52	1.46
3	A	1002	A2E	C9-N10	-2.42	1.34	1.38
2	A	1059	NAG	C6-C5	2.35	1.59	1.51
2	A	1416	NAG	O5-C5	2.33	1.48	1.43
2	B	1592	NAG	C4-C3	2.28	1.58	1.52
2	B	1592	NAG	C2-N2	2.28	1.50	1.46
2	A	1416	NAG	C4-C5	2.25	1.57	1.53
3	B	1001	A2E	C7-C8	2.23	1.40	1.35
3	A	1002	A2E	C7-C8	2.16	1.40	1.35
2	A	1416	NAG	C1-C2	2.16	1.55	1.52
3	A	1002	A2E	C6-C5	2.11	1.53	1.49
3	A	1002	A2E	C8-C9	-2.02	1.39	1.43

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1059	NAG	C1-O5-C5	9.01	124.25	112.19
2	A	1059	NAG	O5-C5-C6	8.84	124.86	107.66
3	B	1001	A2E	C36-C35-C34	-8.08	109.59	120.40
2	A	1457	NAG	C1-O5-C5	7.10	121.70	112.19
3	B	1001	A2E	C35-C34-C28	-7.05	110.45	120.09
3	B	1001	A2E	C35-C36-C37	-6.59	111.59	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	A2E	C26-N27-C28	6.49	125.36	117.67
2	B	1592	NAG	C1-O5-C5	5.65	119.76	112.19
3	A	1002	A2E	C36-C37-C29	-5.48	113.51	120.91
2	B	4162	NAG	C1-O5-C5	5.13	119.06	112.19
3	A	1002	A2E	C32-C33-C26	5.12	121.45	113.48
3	A	1002	A2E	C35-C36-C37	-5.03	113.67	120.40
2	A	1457	NAG	C1-C2-N2	-4.63	103.14	110.43
3	A	1002	A2E	C26-N27-C28	4.63	123.15	117.67
3	B	1001	A2E	C36-C37-C29	-4.51	114.82	120.91
3	A	1002	A2E	C36-C35-C34	-4.49	114.39	120.40
2	B	1592	NAG	O7-C7-C8	-4.48	114.08	122.05
3	B	1001	A2E	C32-C33-C26	4.41	120.34	113.48
2	B	1592	NAG	O6-C6-C5	4.34	126.11	111.33
3	A	1002	A2E	C35-C34-C28	-4.29	114.23	120.09
2	B	1592	NAG	C4-C3-C2	4.26	117.27	111.02
2	A	1059	NAG	O6-C6-C5	4.21	125.68	111.33
2	A	1059	NAG	O3-C3-C2	4.16	118.04	109.40
2	A	1457	NAG	O5-C1-C2	4.16	117.72	111.29
3	A	1002	A2E	C31-C30-C25	4.14	121.25	112.84
2	B	4162	NAG	O5-C1-C2	-3.95	105.17	111.29
2	A	1416	NAG	O5-C5-C6	3.91	115.26	107.66
3	B	1001	A2E	C31-C30-C25	3.90	120.78	112.84
2	B	1592	NAG	C8-C7-N2	3.86	122.52	116.12
2	B	4162	NAG	O4-C4-C5	3.85	118.80	109.32
3	A	1002	A2E	C6-C5-C4	-3.77	119.48	123.50
2	A	1457	NAG	O5-C5-C6	3.76	114.99	107.66
3	B	1001	A2E	C6-C5-N10	3.65	120.66	115.46
2	B	4162	NAG	C1-C2-N2	3.62	116.13	110.43
2	B	1592	NAG	C1-C2-N2	3.53	116.00	110.43
3	B	1001	A2E	C34-C28-C29	3.53	122.94	119.13
3	B	1001	A2E	C25-C26-N27	-3.45	121.22	123.66
2	B	1592	NAG	O3-C3-C2	-3.38	102.38	109.40
3	A	1002	A2E	C25-C26-N27	-3.37	121.27	123.66
3	A	1002	A2E	C6-C5-N10	3.30	120.16	115.46
3	B	1001	A2E	C29-C24-N23	3.27	132.04	121.86
3	B	1001	A2E	C6-C5-C4	-3.24	120.04	123.50
2	A	1416	NAG	O4-C4-C5	3.24	117.30	109.32
2	B	1592	NAG	O4-C4-C3	3.21	117.95	110.38
2	B	4162	NAG	O5-C5-C6	3.11	113.71	107.66
2	A	1457	NAG	O6-C6-C5	2.97	121.45	111.33
3	A	1002	A2E	C1-C2-C3	2.97	114.88	110.97
2	A	1416	NAG	C1-C2-N2	2.92	115.03	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	A2E	C1-C2-C3	2.90	114.78	110.97
2	B	1592	NAG	O5-C5-C6	2.88	113.27	107.66
2	A	1059	NAG	C2-N2-C7	2.87	126.75	122.90
3	A	1002	A2E	O11-C9-C8	-2.86	120.23	125.16
2	B	4162	NAG	O4-C4-C3	2.80	116.98	110.38
3	A	1002	A2E	C24-C25-C26	2.80	120.40	118.68
2	A	1059	NAG	O5-C1-C2	-2.78	106.99	111.29
2	A	1457	NAG	C4-C3-C2	2.77	115.08	111.02
3	B	1001	A2E	C8-C9-N10	2.76	118.67	114.80
3	B	1001	A2E	O11-C9-C8	-2.74	120.44	125.16
3	A	1002	A2E	C33-C26-C25	-2.72	118.62	121.40
2	A	1457	NAG	C2-N2-C7	2.69	126.50	122.90
2	B	1592	NAG	O4-C4-C5	2.51	115.52	109.32
2	B	1592	NAG	C3-C4-C5	2.51	114.79	110.23
2	A	1416	NAG	O3-C3-C4	-2.37	104.78	110.38
3	A	1002	A2E	C30-C25-C26	-2.29	118.75	120.90
3	A	1002	A2E	C8-C9-N10	2.29	118.00	114.80
2	A	1059	NAG	O4-C4-C5	2.25	114.86	109.32
2	A	1457	NAG	O4-C4-C5	2.24	114.85	109.32
3	A	1002	A2E	C7-C4-C5	-2.23	115.69	117.26
2	B	1592	NAG	O3-C3-C4	-2.21	105.16	110.38
3	A	1002	A2E	C29-C24-N23	2.20	128.71	121.86
3	A	1002	A2E	C33-C26-N27	2.17	120.11	116.75
3	B	1001	A2E	C30-C25-C26	-2.06	118.97	120.90

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	A2E	C4-C3-N12-C13
3	A	1002	A2E	C2-C3-N12-C13
2	B	4162	NAG	O5-C5-C6-O6
2	A	1416	NAG	O5-C5-C6-O6
2	A	1059	NAG	C4-C5-C6-O6
2	B	1592	NAG	C4-C5-C6-O6
2	A	1457	NAG	C8-C7-N2-C2
3	B	1001	A2E	C20-C21-C22-N23
2	A	1457	NAG	O5-C5-C6-O6
2	A	1457	NAG	C4-C5-C6-O6
2	A	1457	NAG	O7-C7-N2-C2
2	B	4162	NAG	C4-C5-C6-O6
2	A	1416	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	1002	A2E	C16-C17-C18-C19
3	A	1002	A2E	C15-C16-C17-C18
3	A	1002	A2E	C20-C21-C22-N23
3	B	1001	A2E	C16-C17-C18-C19
3	B	1001	A2E	C2-C3-N12-C13
2	B	1592	NAG	O5-C5-C6-O6
2	A	1059	NAG	O5-C5-C6-O6
3	B	1001	A2E	C17-C18-C19-C20
3	A	1002	A2E	C21-C22-N23-C24
3	A	1002	A2E	C14-C15-C16-C17
3	B	1001	A2E	C29-C24-N23-C22
3	A	1002	A2E	C19-C20-C21-C22
3	A	1002	A2E	C13-C14-C15-C16
3	B	1001	A2E	C15-C16-C17-C18
3	B	1001	A2E	C13-C14-C15-C16
3	A	1002	A2E	C14-C13-N12-C3
3	B	1001	A2E	N12-C13-C14-C15
3	A	1002	A2E	C17-C18-C19-C20
3	B	1001	A2E	C21-C22-N23-C24
3	B	1001	A2E	C4-C3-N12-C13
3	B	1001	A2E	C25-C24-N23-C22
3	B	1001	A2E	C14-C13-N12-C3
3	B	1001	A2E	C19-C20-C21-C22
3	A	1002	A2E	C29-C24-N23-C22

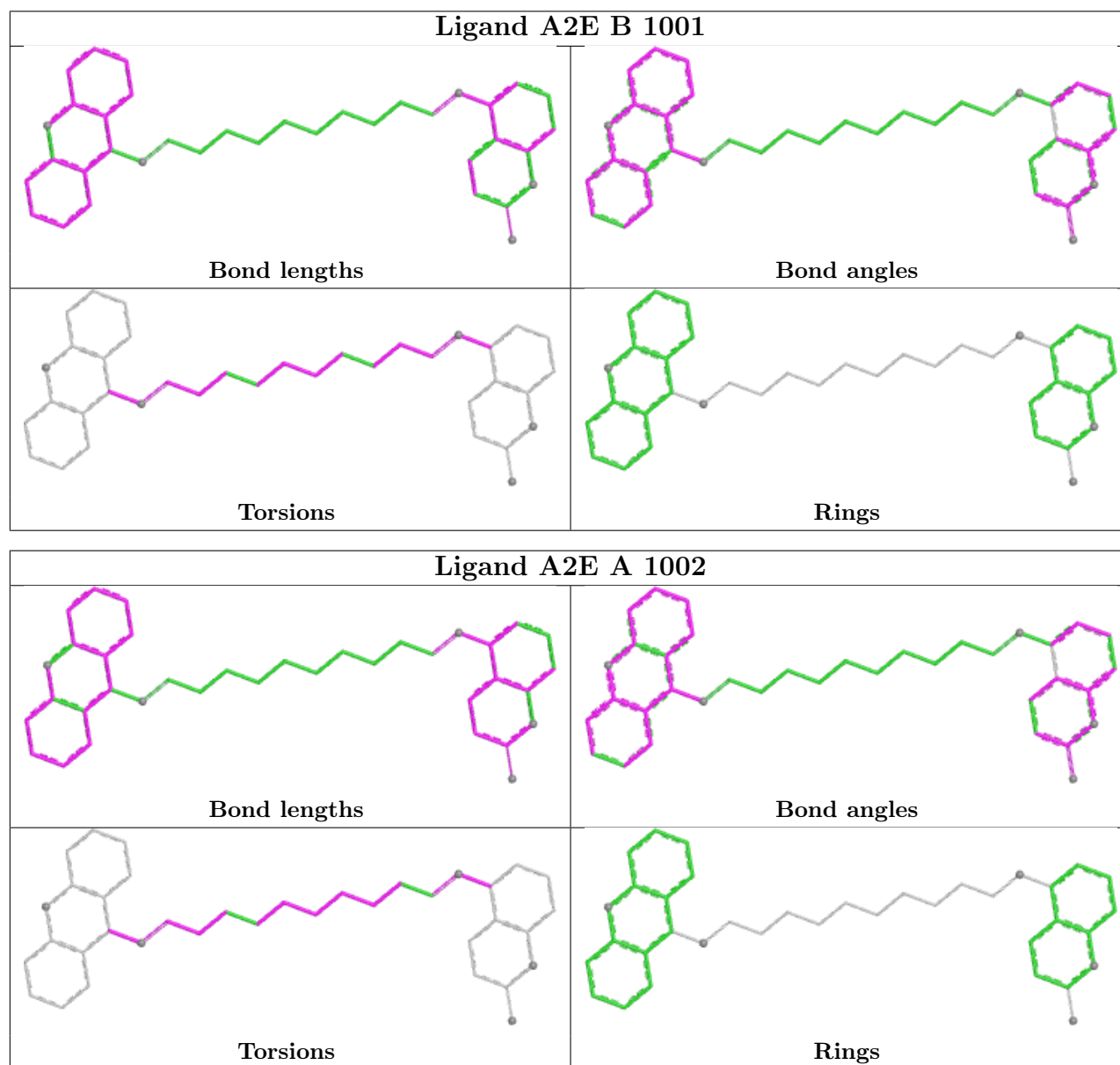
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	A2E	1	0
3	A	1002	A2E	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.



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	528/543 (97%)	-0.13	4 (0%) 82 84	15, 25, 38, 53	0
1	B	528/543 (97%)	-0.17	4 (0%) 82 84	12, 24, 38, 63	0
All	All	1056/1086 (97%)	-0.15	8 (0%) 82 84	12, 24, 38, 63	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	485	PRO	5.5
1	B	535	THR	4.3
1	B	485	PRO	3.3
1	B	284	PHE	2.9
1	A	362	HIS	2.7
1	A	284	PHE	2.6
1	B	257	ASN	2.6
1	A	23	LEU	2.3

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.

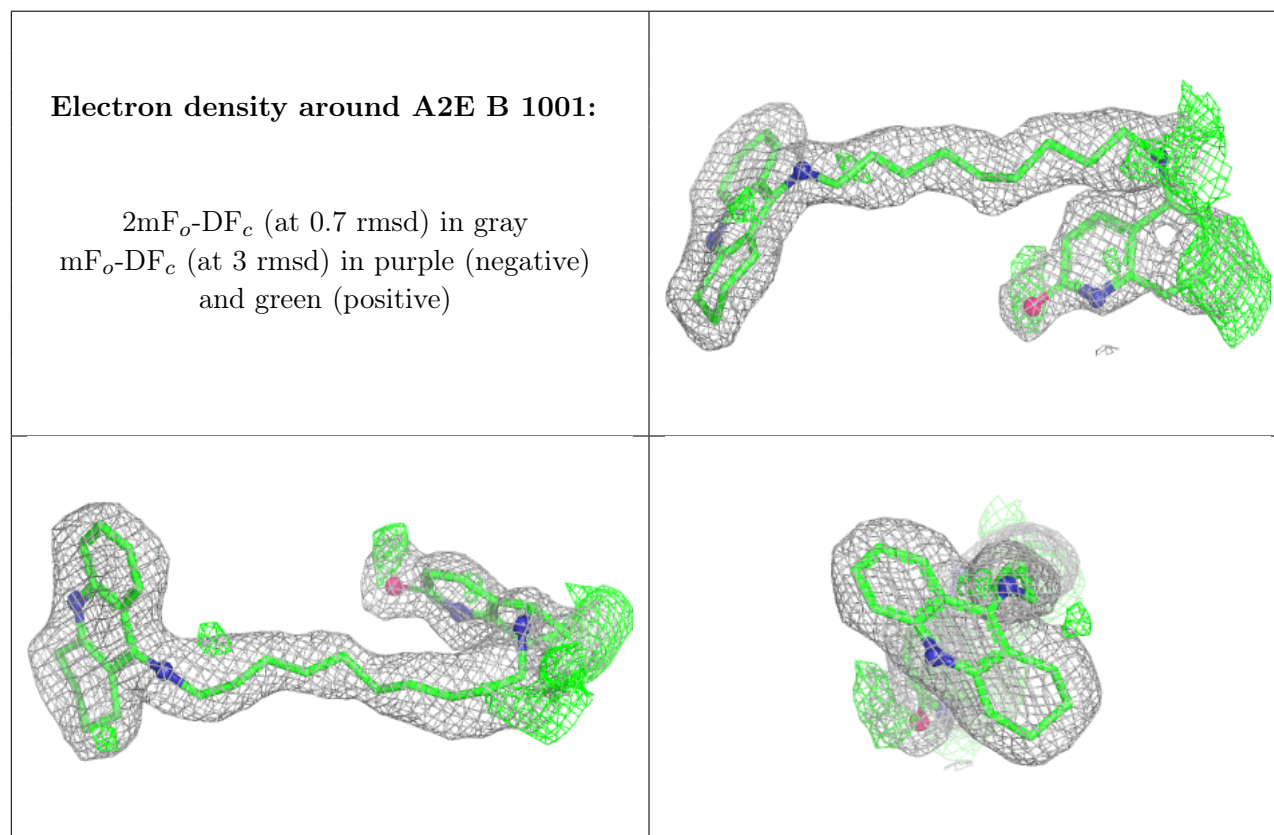
6.4 Ligands [i](#)

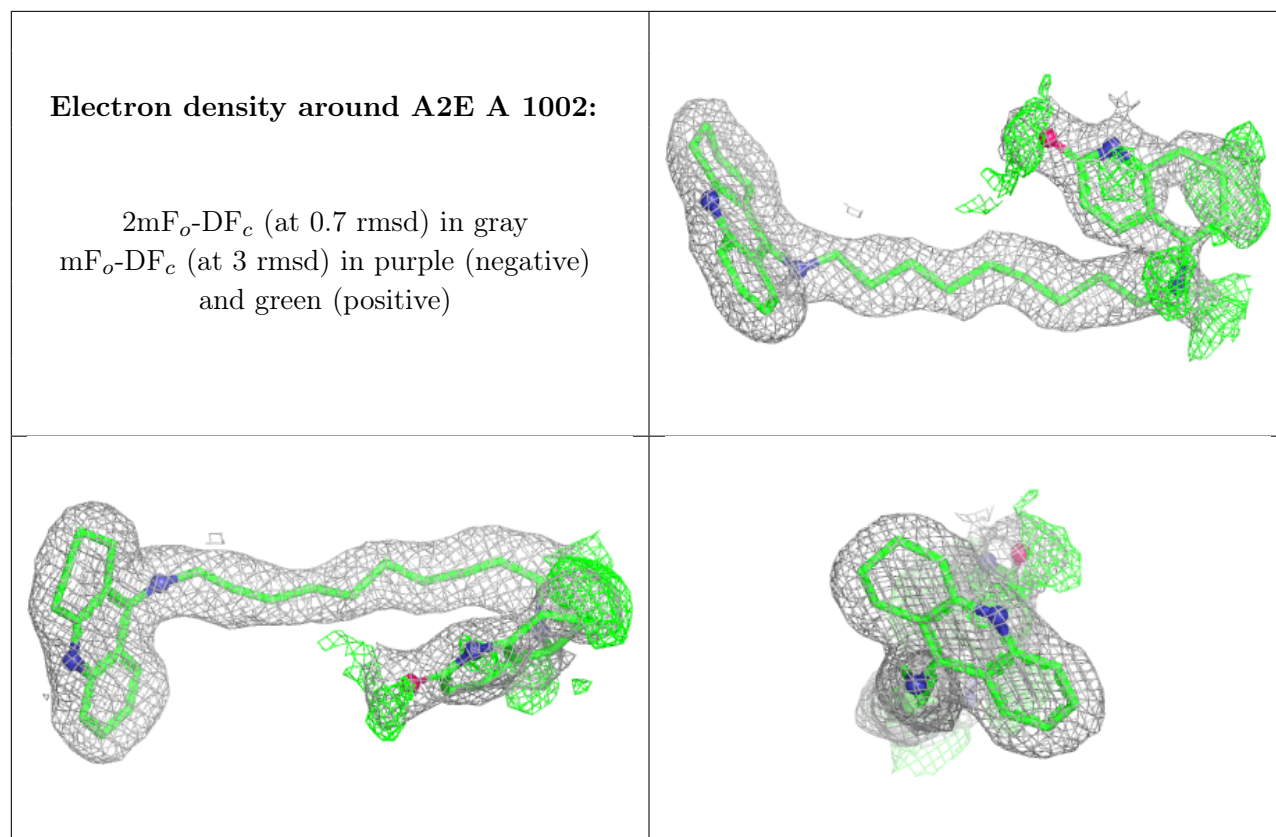
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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($\text{\AA}^2$)	Q<0.9
2	NAG	A	1457	14/15	0.68	0.18	69,75,77,78	0
2	NAG	A	1059	14/15	0.74	0.17	62,68,70,70	0
2	NAG	B	1592	14/15	0.83	0.13	42,46,49,54	0
2	NAG	B	4162	14/15	0.84	0.12	37,42,49,51	0
2	NAG	A	1416	14/15	0.85	0.12	39,48,58,59	0
3	A2E	B	1001	37/37	0.85	0.16	19,27,40,41	12
3	A2E	A	1002	37/37	0.87	0.15	16,25,39,41	12

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.