Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 02:57 pm GMT

PDB ID : 1HK3

Title : Human serum albumin mutant r218p complexed with thyroxine (3,3',5,5'-tetr aiodo-l-thyronine)

Authors : Petitpas, I.; Petersen, C.E.; Ha, C.E.; Bhattacharya, A.A.; Zunszain, P.A.; Ghuman, J.; Bhagavan, N.V.; Curry, S.

Deposited on : 2003-03-05

Resolution : 2.80 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

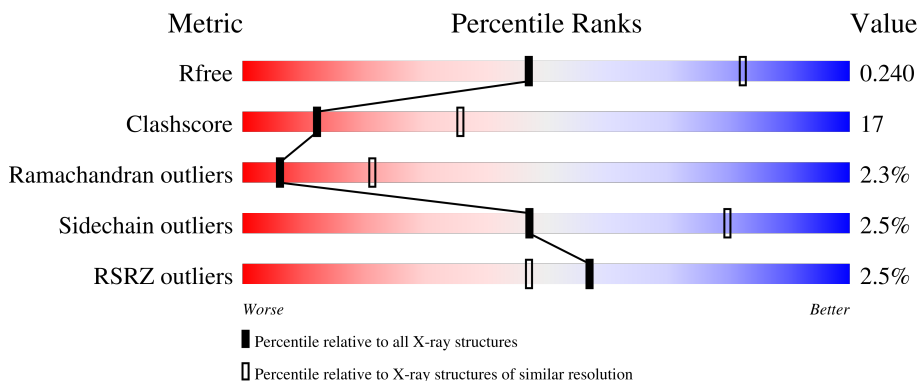|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1　Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
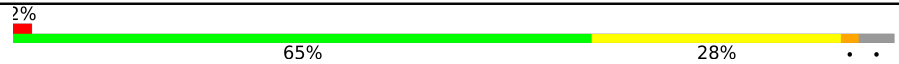*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Rfree		0.240
Clashscore		17
Ramachandran outliers		2.3%
Sidechain outliers		2.5%
RSRZ outliers		2.5%

Worse ... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	585	2%　65%　28%　·　·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4408 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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	4299	2724	721	814	40	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	PRO	ARG	engineered mutation	UNP P02768

- Molecule 2 is 3,5,3',5'-TETRAIODO-L-THYRONINE (three-letter code: T44) (formula: $C_{15}H_{11}I_4NO_4$).
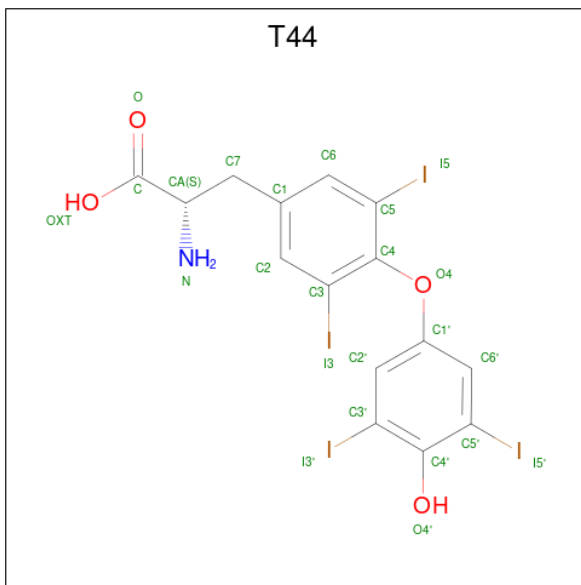
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	I	N	O		
2	A	1	24	15	4	1	4	0	0
2	A	1	24	15	4	1	4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 24	C 15	I 4	N 1	O 4	0	0
2	A	1	Total 24	C 15	I 4	N 1	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total 13	O 13	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: SERUM ALBUMIN
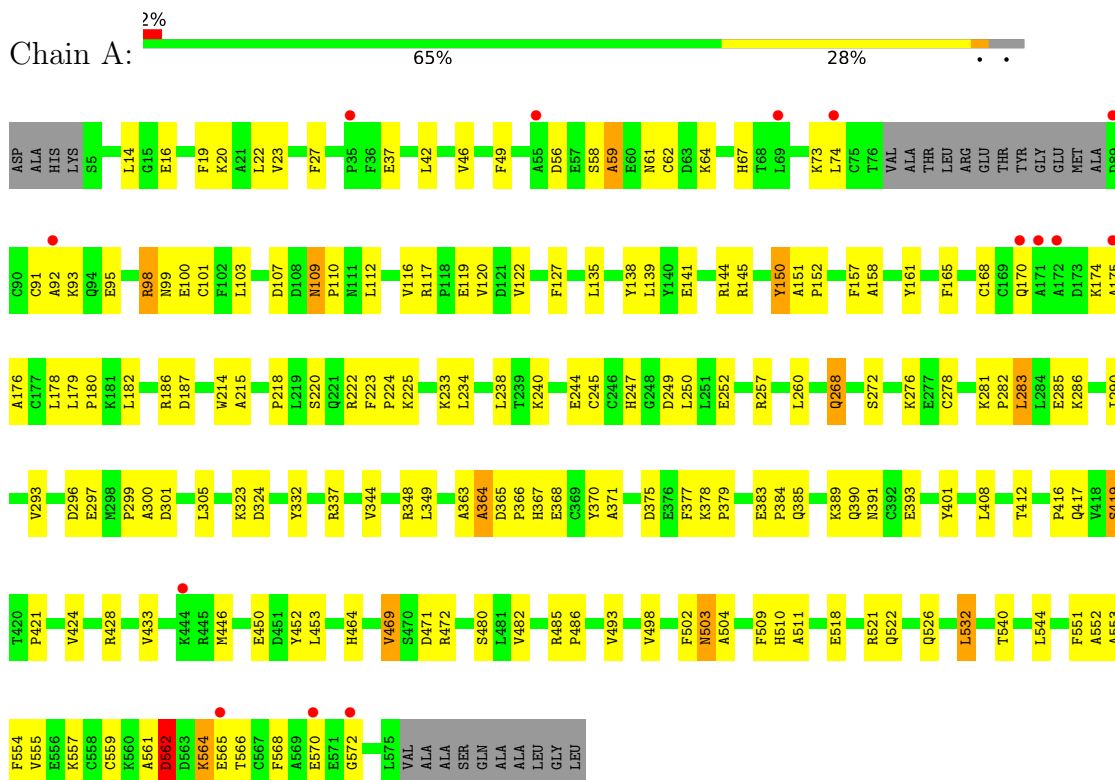
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.33Å 89.28Å 60.53Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	35.12 – 2.80 35.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.9 (35.12-2.80) 95.0 (35.12-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.245 0.197 , 0.240	Depositor DCC
R_{free} test set	700 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å^2)	69.9	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 52.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4408	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: T44

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	0.41	0/4387	0.62	2/5950 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	562	ASP	N-CA-C	-5.27	96.78	111.00
1	A	150	TYR	CB-CG-CD2	-5.21	117.87	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4299	0	4057	144	0
2	A	96	0	16	2	0
3	A	13	0	0	1	0
All	All	4408	0	4073	144	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 17.

All (144) 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:120:VAL:HG21	1:A:175:ALA:HB2	1.53	0.91
1:A:214:TRP:O	1:A:218:PRO:HD3	1.70	0.91
1:A:225:LYS:HD3	1:A:299:PRO:HG3	1.52	0.90
1:A:391:ASN:HB3	2:A:3002:T44:I3	2.45	0.87
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.59	0.85
1:A:561:ALA:HB2	1:A:564:LYS:HE3	1.58	0.84
1:A:518:GLU:O	1:A:522:GLN:HG3	1.79	0.83
1:A:220:SER:HG	1:A:332:TYR:HD1	1.32	0.78
1:A:95:GLU:OE2	1:A:99:ASN:HB2	1.89	0.73
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.71	0.72
1:A:141:GLU:O	1:A:144:ARG:HG2	1.88	0.72
1:A:365:ASP:OD2	1:A:368:GLU:HG2	1.90	0.71
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.73	0.70
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.73	0.70
1:A:19:PHE:O	1:A:23:VAL:HG23	1.93	0.68
1:A:424:VAL:O	1:A:428:ARG:HG3	1.94	0.67
1:A:215:ALA:O	1:A:218:PRO:HD2	1.95	0.67
1:A:552:ALA:O	1:A:555:VAL:HG12	1.95	0.66
1:A:385:GLN:HG3	1:A:446:MET:CE	2.28	0.63
1:A:120:VAL:HG21	1:A:175:ALA:CB	2.27	0.63
1:A:518:GLU:OE2	1:A:521:ARG:NH1	2.31	0.63
1:A:419:SER:OG	1:A:421:PRO:HD2	1.99	0.62
1:A:182:LEU:HD22	1:A:186:ARG:NH2	2.14	0.62
1:A:238:LEU:HD13	1:A:260:LEU:HD21	1.80	0.62
1:A:249:ASP:HB3	1:A:252:GLU:CG	2.30	0.62
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.40	0.61
1:A:225:LYS:CD	1:A:299:PRO:HG3	2.29	0.61
1:A:107:ASP:HB3	1:A:110:PRO:HG3	1.83	0.61
1:A:127:PHE:CD2	1:A:165:PHE:HB3	2.35	0.61
1:A:503:ASN:O	1:A:504:ALA:HB3	2.01	0.60
1:A:103:LEU:HD21	1:A:247:HIS:O	2.00	0.60
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.21	0.59
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.82	0.59
1:A:349:LEU:HD22	1:A:377:PHE:CG	2.37	0.59
1:A:119:GLU:HB2	1:A:122:VAL:HG23	1.83	0.58
1:A:240:LYS:HG2	1:A:244:GLU:OE2	2.03	0.58
1:A:182:LEU:O	1:A:186:ARG:HG2	2.02	0.58
1:A:119:GLU:O	1:A:122:VAL:HB	2.04	0.58
1:A:553:ALA:O	1:A:557:LYS:HG2	2.03	0.58
1:A:161:TYR:HE1	1:A:186:ARG:HH22	1.50	0.58
1:A:268:GLN:OE1	1:A:276:LYS:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:VAL:HG21	1:A:453:LEU:HD21	1.85	0.57
1:A:218:PRO:O	1:A:222:ARG:HG2	2.04	0.57
1:A:27:PHE:CD1	1:A:74:LEU:HD21	2.40	0.56
1:A:532:LEU:HD13	1:A:544:LEU:HD22	1.86	0.56
1:A:278:CYS:O	1:A:281:LYS:HG2	2.06	0.56
1:A:390:GLN:HB2	2:A:3002:T44:I3	2.77	0.55
1:A:348:ARG:HH22	1:A:450:GLU:CD	2.09	0.55
1:A:349:LEU:HD22	1:A:377:PHE:CD1	2.42	0.55
1:A:42:LEU:O	1:A:46:VAL:HG23	2.07	0.54
1:A:559:CYS:C	1:A:561:ALA:N	2.61	0.54
1:A:323:LYS:HG3	1:A:324:ASP:H	1.73	0.54
1:A:323:LYS:HG3	1:A:324:ASP:N	2.23	0.54
1:A:472:ARG:HD3	3:A:2010:HOH:O	2.08	0.53
1:A:14:LEU:HD13	1:A:22:LEU:HD12	1.91	0.53
1:A:433:VAL:HG22	1:A:452:TYR:HD2	1.73	0.53
1:A:305:LEU:HD11	1:A:337:ARG:HD2	1.89	0.53
1:A:234:LEU:O	1:A:238:LEU:HB2	2.08	0.53
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.44	0.53
1:A:127:PHE:CE2	1:A:165:PHE:HB3	2.44	0.52
1:A:502:PHE:CE2	1:A:504:ALA:HB2	2.45	0.52
1:A:91:CYS:C	1:A:93:LYS:H	2.12	0.52
1:A:37:GLU:H	1:A:37:GLU:CD	2.12	0.52
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.92	0.52
1:A:464:HIS:CE1	1:A:469:VAL:H	2.28	0.51
1:A:389:LYS:O	1:A:393:GLU:HG3	2.11	0.51
1:A:135:LEU:O	1:A:138:TYR:HB3	2.10	0.51
1:A:498:VAL:O	1:A:498:VAL:HG23	2.11	0.51
1:A:296:ASP:OD1	1:A:297:GLU:N	2.44	0.50
1:A:42:LEU:HD22	1:A:73:LYS:HB3	1.94	0.50
1:A:367:HIS:O	1:A:371:ALA:HB2	2.12	0.50
1:A:364:ALA:O	1:A:366:PRO:HD3	2.12	0.50
1:A:485:ARG:HD2	1:A:485:ARG:C	2.32	0.50
1:A:559:CYS:C	1:A:561:ALA:H	2.14	0.50
1:A:16:GLU:O	1:A:20:LYS:HG3	2.12	0.49
1:A:56:ASP:C	1:A:58:SER:H	2.15	0.49
1:A:119:GLU:HB2	1:A:122:VAL:CG2	2.41	0.49
1:A:151:ALA:HB2	1:A:250:LEU:HD13	1.94	0.49
1:A:281:LYS:HD3	1:A:285:GLU:HB3	1.94	0.49
1:A:247:HIS:HD1	1:A:249:ASP:CG	2.15	0.49
1:A:566:THR:O	1:A:570:GLU:N	2.35	0.49
1:A:220:SER:OG	1:A:332:TYR:HD1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:HIS:NE2	1:A:249:ASP:OD1	2.46	0.48
1:A:272:SER:HA	1:A:296:ASP:OD2	2.13	0.48
1:A:433:VAL:HG21	1:A:453:LEU:CD2	2.43	0.48
1:A:290:ILE:O	1:A:293:VAL:HG22	2.13	0.47
1:A:348:ARG:HG3	1:A:482:VAL:CG1	2.44	0.47
1:A:433:VAL:CG2	1:A:452:TYR:HD2	2.28	0.47
1:A:485:ARG:NH1	1:A:486:PRO:HA	2.29	0.47
1:A:138:TYR:CE2	1:A:158:ALA:HA	2.49	0.47
1:A:186:ARG:N	1:A:186:ARG:HD3	2.29	0.47
1:A:412:THR:O	1:A:416:PRO:HG3	2.14	0.47
1:A:168:CYS:HB2	1:A:178:LEU:HD13	1.98	0.46
1:A:485:ARG:HB3	1:A:486:PRO:CD	2.38	0.46
1:A:561:ALA:HB2	1:A:564:LYS:CE	2.38	0.46
1:A:145:ARG:HH11	1:A:145:ARG:HG3	1.81	0.46
1:A:370:TYR:C	1:A:370:TYR:CD1	2.89	0.45
1:A:401:TYR:HE1	1:A:522:GLN:HB3	1.81	0.45
1:A:493:VAL:HG23	1:A:493:VAL:O	2.16	0.45
1:A:305:LEU:CD1	1:A:337:ARG:HD2	2.46	0.45
1:A:568:PHE:O	1:A:572:GLY:HA3	2.17	0.44
1:A:401:TYR:CE1	1:A:522:GLN:HB3	2.53	0.44
1:A:49:PHE:HZ	1:A:61:ASN:HB2	1.82	0.44
1:A:19:PHE:CD1	1:A:19:PHE:C	2.91	0.44
1:A:170:GLN:HG2	1:A:170:GLN:O	2.18	0.43
1:A:109:ASN:N	1:A:110:PRO:HD3	2.33	0.43
1:A:116:VAL:HG22	1:A:117:ARG:N	2.34	0.43
1:A:286:LYS:O	1:A:290:ILE:CG1	2.67	0.43
1:A:503:ASN:O	1:A:504:ALA:CB	2.66	0.43
1:A:252:GLU:OE1	1:A:252:GLU:N	2.42	0.43
1:A:98:ARG:O	1:A:101:CYS:HB3	2.19	0.43
1:A:378:LYS:CB	1:A:379:PRO:HD3	2.48	0.43
1:A:551:PHE:O	1:A:554:PHE:HB3	2.19	0.43
1:A:19:PHE:CE1	1:A:23:VAL:HG21	2.54	0.42
1:A:99:ASN:C	1:A:101:CYS:H	2.22	0.42
1:A:233:LYS:C	1:A:233:LYS:HD3	2.39	0.42
1:A:385:GLN:HG3	1:A:446:MET:HE2	2.00	0.42
1:A:561:ALA:HB1	1:A:562:ASP:H	1.45	0.42
1:A:95:GLU:OE1	1:A:98:ARG:HD2	2.18	0.42
1:A:509:PHE:CD2	1:A:565:GLU:HG2	2.55	0.42
1:A:408:LEU:HA	1:A:408:LEU:HD23	1.77	0.42
1:A:282:PRO:O	1:A:283:LEU:C	2.58	0.42
1:A:174:LYS:C	1:A:176:ALA:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ALA:O	1:A:562:ASP:CB	2.67	0.42
1:A:348:ARG:HG3	1:A:482:VAL:HG12	2.02	0.41
1:A:56:ASP:C	1:A:58:SER:N	2.73	0.41
1:A:99:ASN:C	1:A:101:CYS:N	2.72	0.41
1:A:344:VAL:HG21	1:A:450:GLU:HG2	2.02	0.41
1:A:100:GLU:HA	1:A:100:GLU:OE1	2.20	0.41
1:A:281:LYS:HB2	1:A:282:PRO:HD2	2.01	0.41
1:A:152:PRO:HB2	1:A:257:ARG:HH11	1.85	0.41
1:A:238:LEU:HD13	1:A:260:LEU:CD2	2.49	0.41
1:A:222:ARG:C	1:A:224:PRO:HD3	2.41	0.41
1:A:249:ASP:HB3	1:A:252:GLU:OE2	2.21	0.41
1:A:383:GLU:N	1:A:384:PRO:CD	2.83	0.41
1:A:510:HIS:O	1:A:511:ALA:C	2.59	0.41
1:A:249:ASP:O	1:A:252:GLU:HG2	2.21	0.41
1:A:555:VAL:HG23	1:A:568:PHE:CZ	2.56	0.41
1:A:110:PRO:HB2	1:A:112:LEU:HG	2.04	0.40
1:A:103:LEU:HD11	1:A:247:HIS:CD2	2.56	0.40
1:A:223:PHE:HD1	1:A:272:SER:HB2	1.86	0.40
1:A:417:GLN:H	1:A:417:GLN:CD	2.25	0.40
1:A:138:TYR:OH	1:A:157:PHE:HB3	2.21	0.40
1:A:555:VAL:HG23	1:A:568:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/585 (95%)	496 (89%)	46 (8%)	13 (2%)	6	21

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	ASP
1	A	301	ASP
1	A	59	ALA
1	A	64	LYS
1	A	92	ALA
1	A	564	LYS
1	A	150	TYR
1	A	268	GLN
1	A	300	ALA
1	A	363	ALA
1	A	364	ALA
1	A	283	LEU
1	A	469	VAL

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	446/511 (87%)	435 (98%)	11 (2%)	47	80

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

Mol	Chain	Res	Type
1	A	98	ARG
1	A	109	ASN
1	A	187	ASP
1	A	245	CYS
1	A	375	ASP
1	A	419	SER
1	A	471	ASP
1	A	480	SER
1	A	503	ASN
1	A	532	LEU
1	A	540	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	109	ASN
1	A	196	GLN
1	A	385	GLN
1	A	464	HIS
1	A	483	ASN
1	A	503	ASN
1	A	510	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	T44	A	3004	-	24,25,25	1.34	5 (20%)	35,36,36	1.03	1 (2%)
2	T44	A	3002	-	24,25,25	1.47	7 (29%)	35,36,36	0.98	0
2	T44	A	3003	-	24,25,25	1.34	3 (12%)	35,36,36	1.18	4 (11%)
2	T44	A	3001	-	24,25,25	1.16	2 (8%)	35,36,36	1.11	1 (2%)

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	T44	A	3004	-	-	2/12/12/12	0/2/2/2
2	T44	A	3002	-	-	4/12/12/12	0/2/2/2
2	T44	A	3003	-	-	0/12/12/12	0/2/2/2
2	T44	A	3001	-	-	5/12/12/12	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3004	T44	C6'-C1'	3.47	1.45	1.38
2	A	3003	T44	O4'-C4'	-3.24	1.29	1.37
2	A	3002	T44	O4-C1'	2.71	1.45	1.39
2	A	3003	T44	C2'-C1'	2.64	1.43	1.38
2	A	3002	T44	C4'-C3'	2.59	1.46	1.40
2	A	3004	T44	O4'-C4'	-2.53	1.31	1.37
2	A	3003	T44	C4'-C3'	2.46	1.45	1.40
2	A	3002	T44	C6'-C1'	2.40	1.43	1.38
2	A	3002	T44	C6-C1	2.35	1.43	1.39
2	A	3001	T44	C4'-C3'	2.29	1.45	1.40
2	A	3002	T44	C2'-C3'	2.23	1.44	1.39
2	A	3001	T44	OXT-C	-2.21	1.23	1.30
2	A	3002	T44	O4'-C4'	-2.13	1.32	1.37
2	A	3004	T44	C4'-C3'	2.11	1.44	1.40
2	A	3002	T44	OXT-C	-2.06	1.23	1.30
2	A	3004	T44	OXT-C	-2.06	1.23	1.30
2	A	3004	T44	C6-C1	2.01	1.42	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3003	T44	C1'-O4-C4	3.75	124.52	118.48
2	A	3004	T44	C1-C7-CA	2.70	119.75	114.13
2	A	3001	T44	C4'-C3'-I3'	-2.55	115.49	119.42
2	A	3003	T44	C6'-C5'-C4'	2.32	125.67	121.21
2	A	3003	T44	C4'-C5'-I5'	-2.25	115.95	119.42
2	A	3003	T44	C2-C3-I3	2.15	122.58	118.61

There are no chirality outliers.
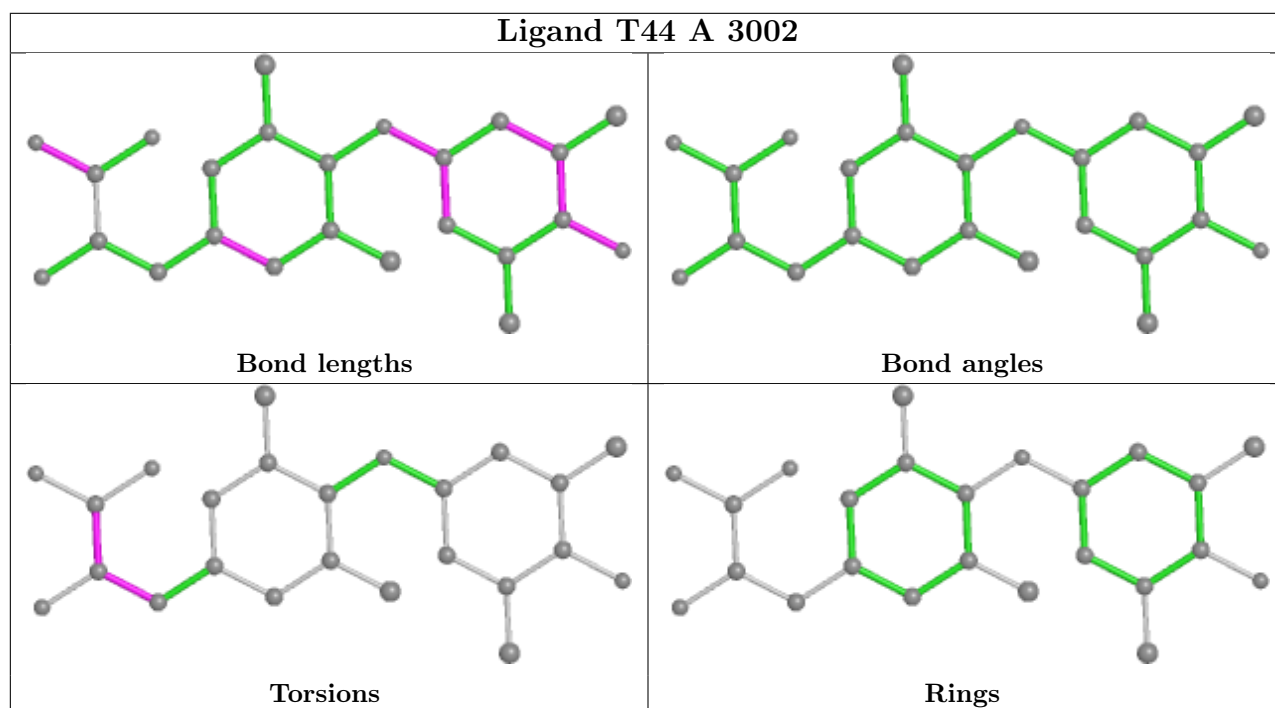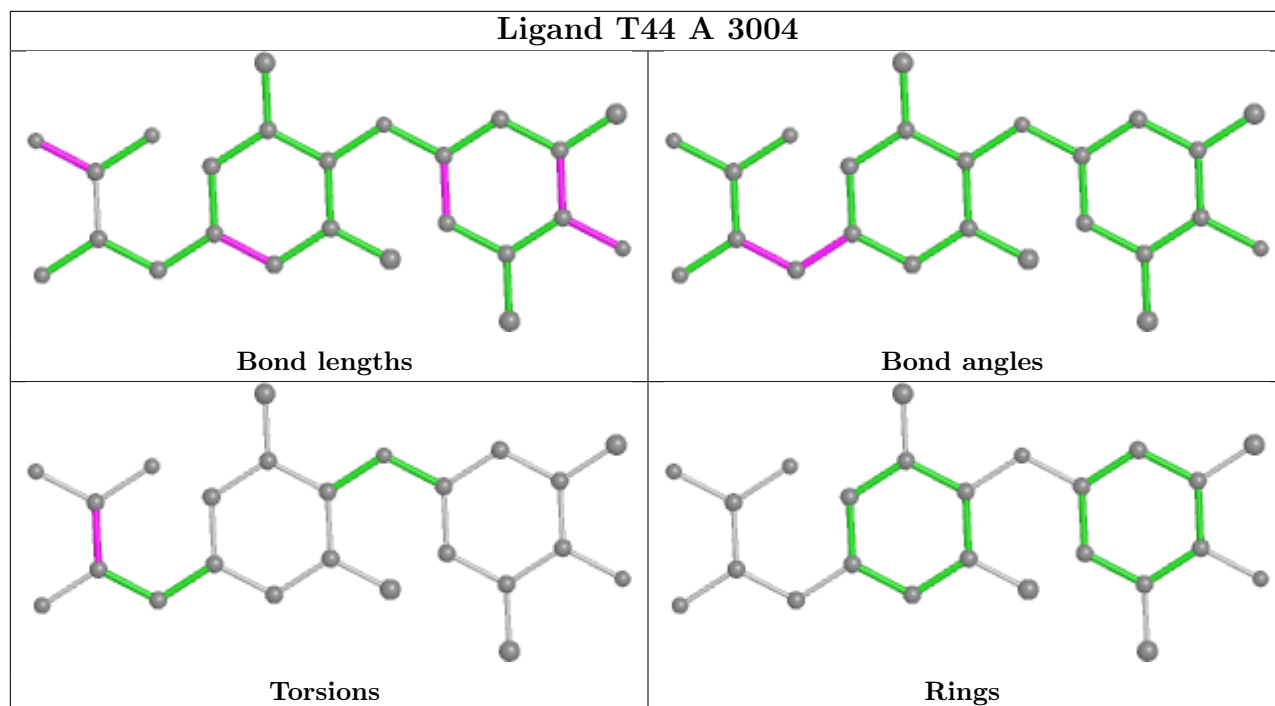
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	T44	C1-C7-CA-C
2	A	3002	T44	C1-C7-CA-C
2	A	3004	T44	O-C-CA-N
2	A	3001	T44	OXT-C-CA-N
2	A	3002	T44	OXT-C-CA-N
2	A	3001	T44	C1-C7-CA-N
2	A	3002	T44	C1-C7-CA-N
2	A	3004	T44	OXT-C-CA-N
2	A	3001	T44	O-C-CA-N
2	A	3002	T44	O-C-CA-N
2	A	3001	T44	OXT-C-CA-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3002	T44	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand T44 A 3004

Bond lengths

Bond angles

Torsions

Rings

Ligand T44 A 3002

Bond lengths

Bond angles

Torsions

Rings

Ligand T44 A 3003

Bond lengths

Bond angles

Torsions

Rings

Ligand T44 A 3001

Bond lengths

Bond angles

Torsions

Rings
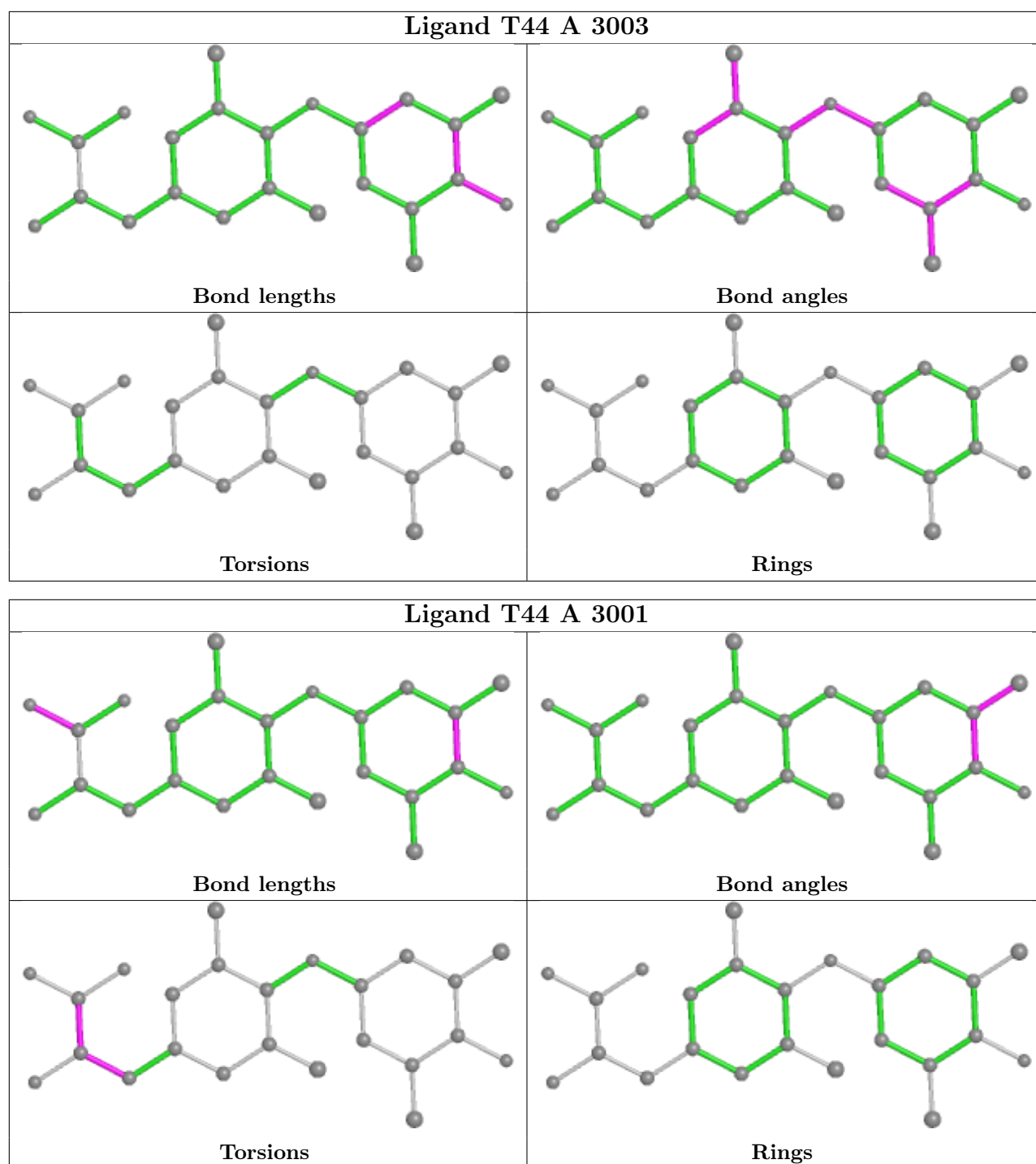
5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	559/585 (95%)	-0.26	14 (2%)	57	47	43, 74, 121, 130	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	ALA	4.2
1	A	171	ALA	3.7
1	A	170	GLN	3.3
1	A	92	ALA	3.0
1	A	175	ALA	2.8
1	A	55	ALA	2.7
1	A	74	LEU	2.5
1	A	444	LYS	2.5
1	A	565	GLU	2.4
1	A	572	GLY	2.3
1	A	570	GLU	2.2
1	A	35	PRO	2.2
1	A	89	ASP	2.1
1	A	69	LEU	2.1

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

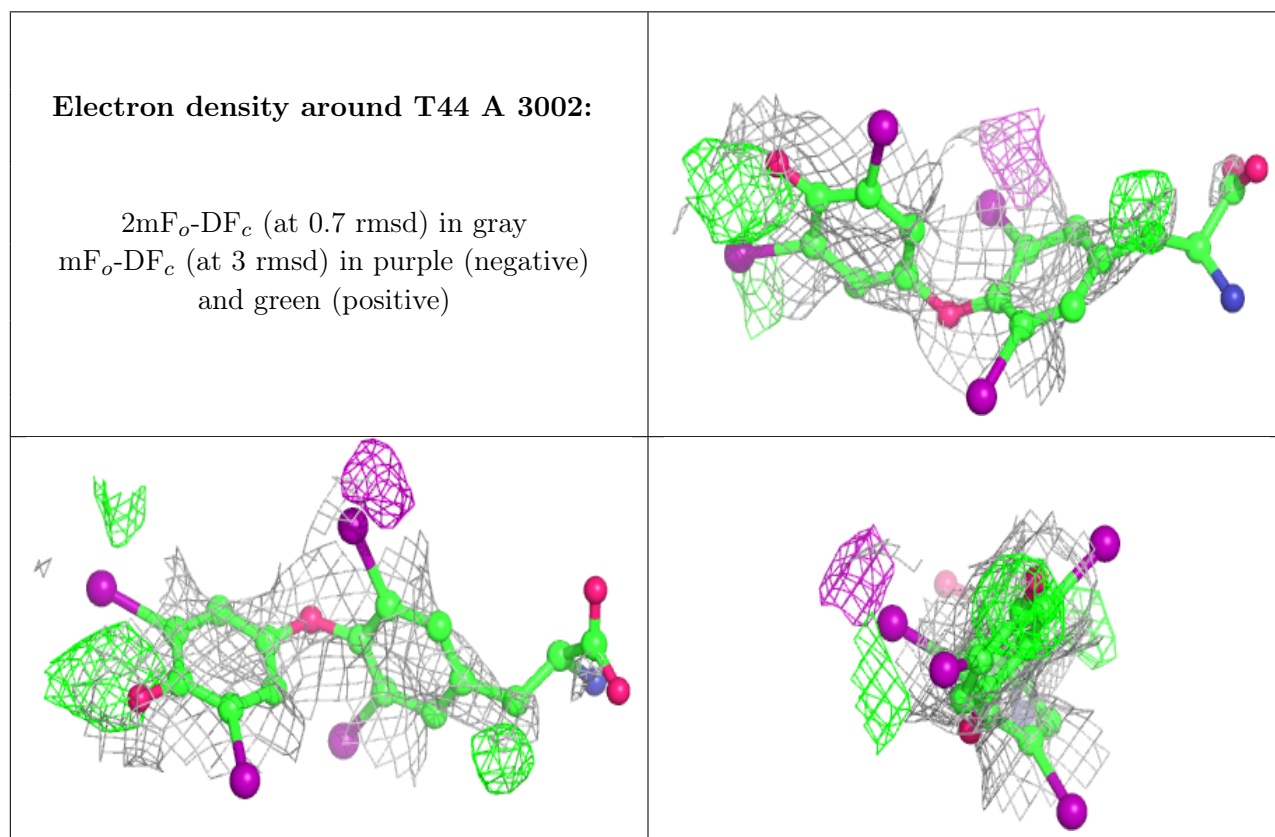There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	T44	A	3002	24/24	0.97	0.21	55,70,84,87	24
2	T44	A	3001	24/24	0.99	0.18	60,64,73,77	0
2	T44	A	3003	24/24	0.99	0.12	56,64,66,68	0
2	T44	A	3004	24/24	0.99	0.16	62,76,83,84	24

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.
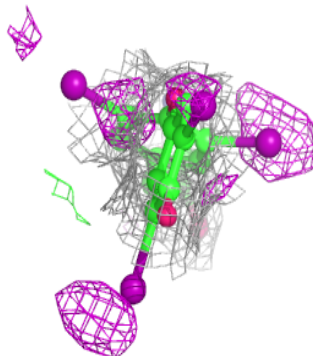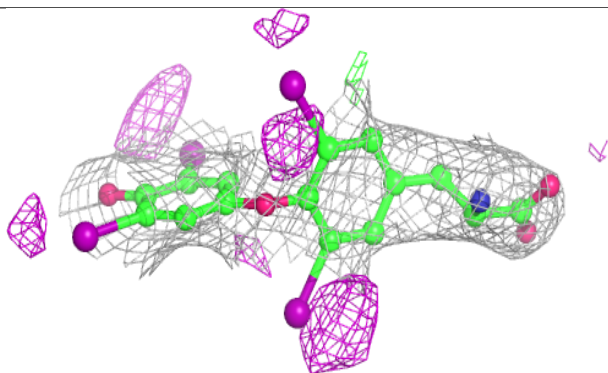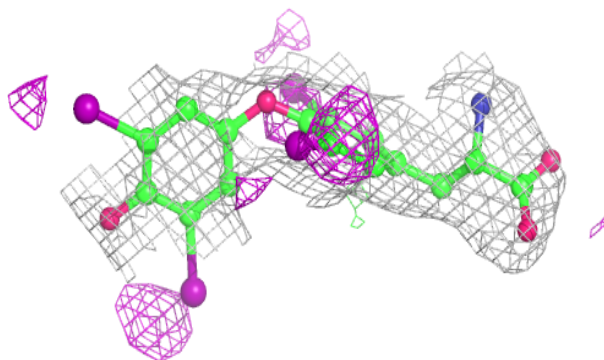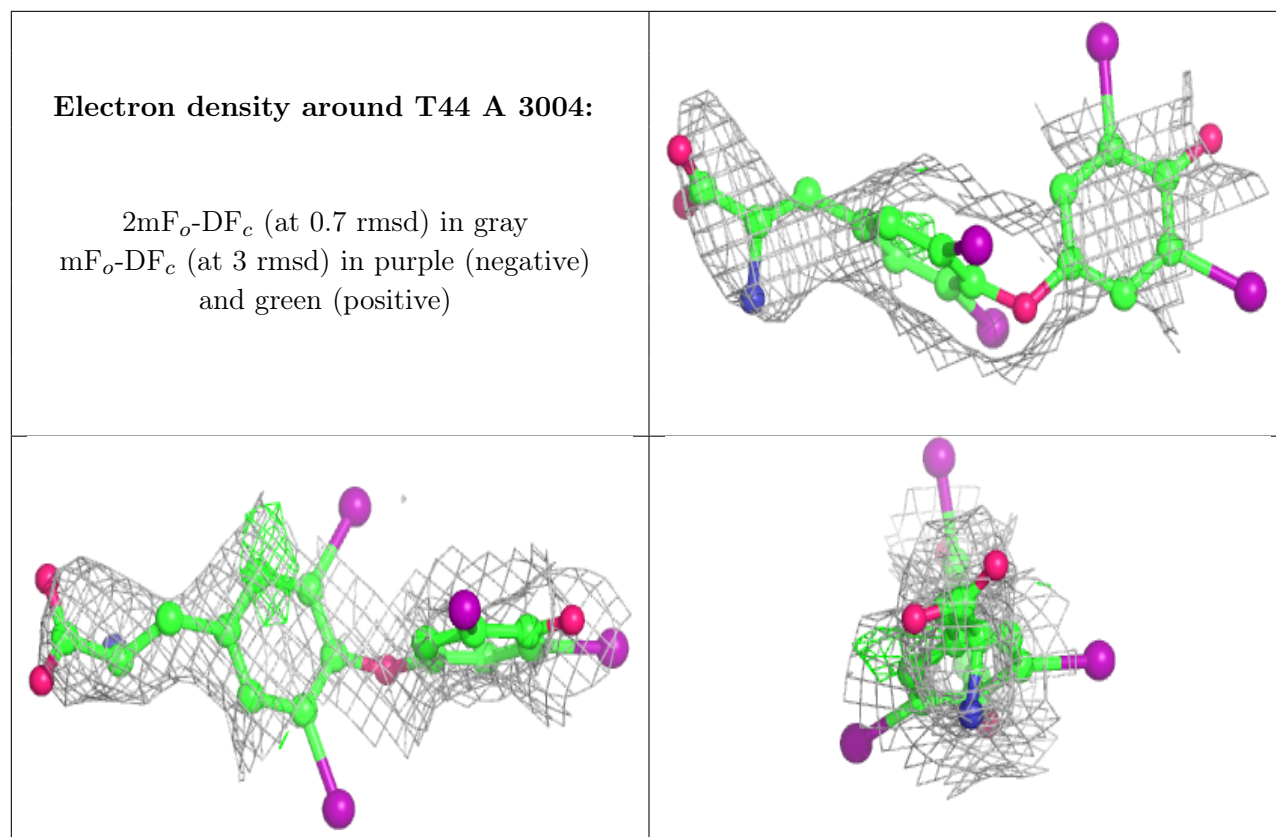

Electron density around T44 A 3002:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around T44 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)
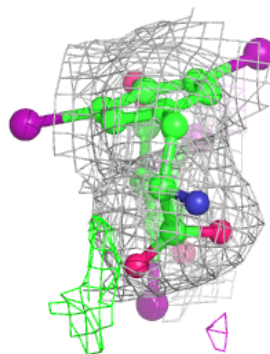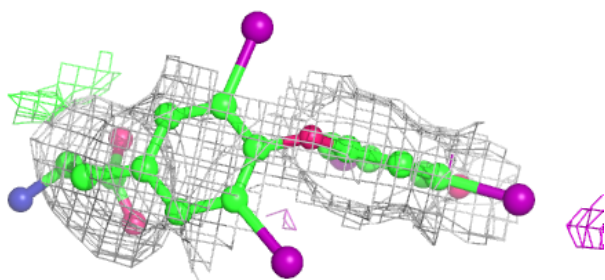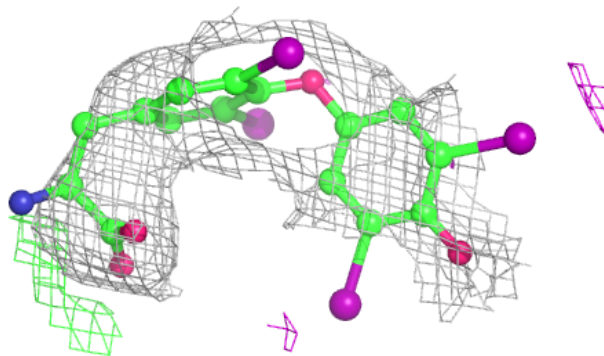
Electron density around T44 A 3003:

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 T44 A 3004:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.