Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:09 pm BST

PDB ID	:	1XNX
Title	:	Crystal structure of constitutive androstane receptor
Authors	:	Fernandez, E.
Deposited on	:	2004-10-05
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

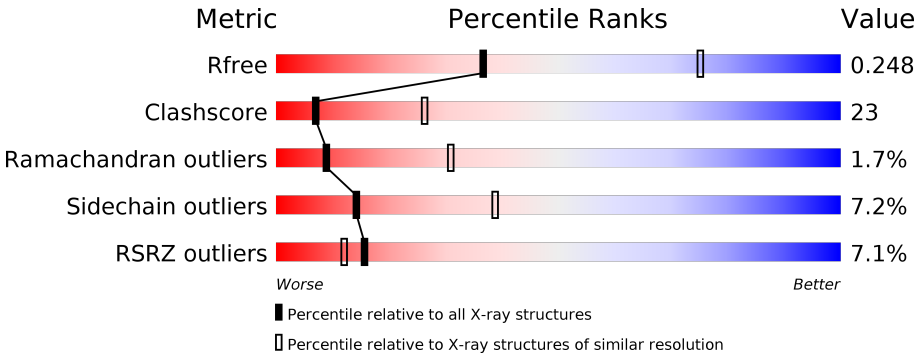
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	256	3% 57% 30% • 9%
1	B	256	10% 43% 41% 7% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3863 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.

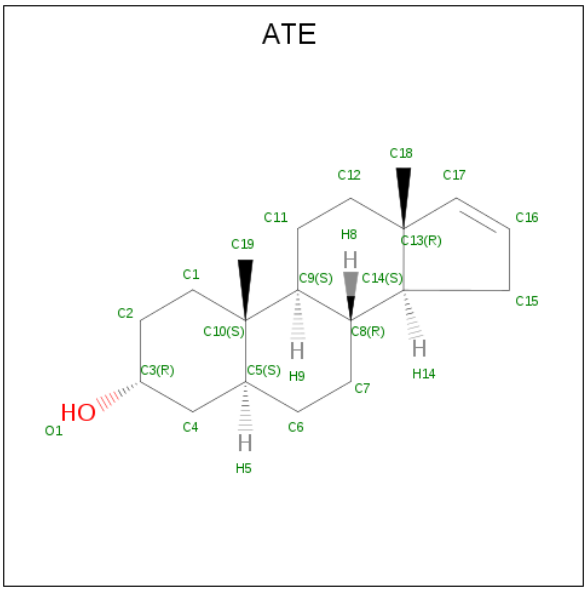
- Molecule 1 is a protein called constitutive androstane receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1901	1229	323	338	11			
1	B	232	Total	C	N	O	S	0	0	0
			1889	1225	319	333	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	HIS	-	EXPRESSION TAG	UNP O35627
A	104	HIS	-	EXPRESSION TAG	UNP O35627
A	105	HIS	-	EXPRESSION TAG	UNP O35627
A	106	HIS	-	EXPRESSION TAG	UNP O35627
A	107	HIS	-	EXPRESSION TAG	UNP O35627
A	108	HIS	-	EXPRESSION TAG	UNP O35627
B	103	HIS	-	EXPRESSION TAG	UNP O35627
B	104	HIS	-	EXPRESSION TAG	UNP O35627
B	105	HIS	-	EXPRESSION TAG	UNP O35627
B	106	HIS	-	EXPRESSION TAG	UNP O35627
B	107	HIS	-	EXPRESSION TAG	UNP O35627
B	108	HIS	-	EXPRESSION TAG	UNP O35627

- Molecule 2 is 16,17-ANDROSTENE-3-OL (three-letter code: ATE) (formula: $C_{19}H_{30}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 20 19 1	0	0
2	B	1	Total C O 20 19 1	0	0

- Molecule 3 is water.

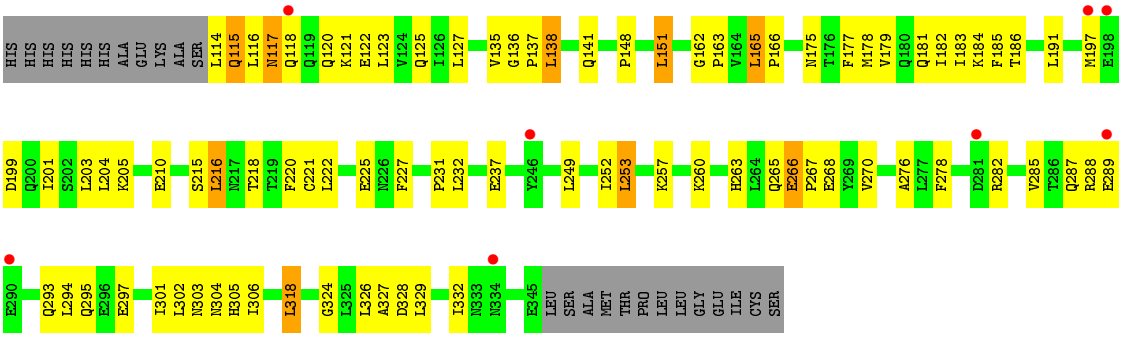
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	18	Total O 18 18	0	0
3	B	15	Total O 15 15	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

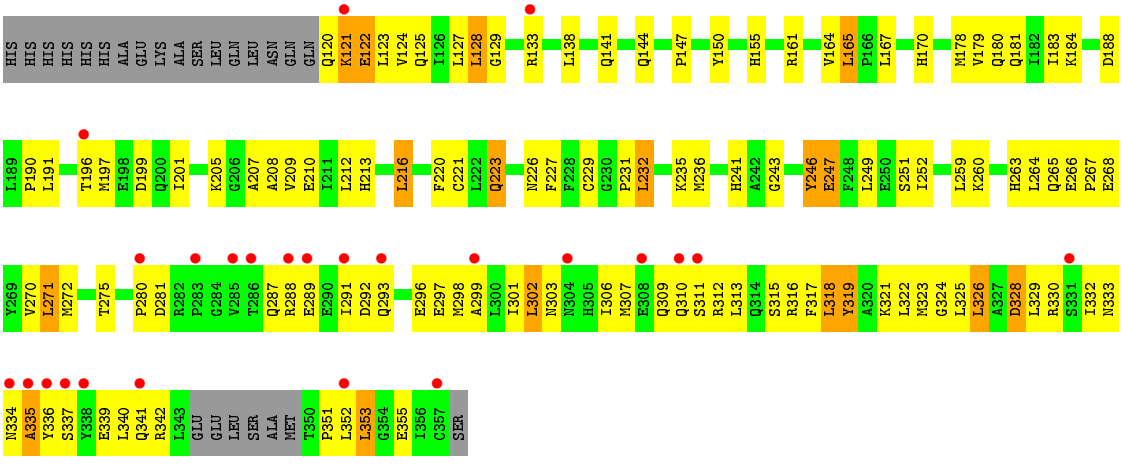
- Molecule 1: constitutive androstane receptor

Chain A:



- Molecule 1: constitutive androstane receptor

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	60.35Å 155.04Å 134.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.90 29.54 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.55-2.90) 100.0 (29.54-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.72 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.288 0.203 , 0.248	Depositor DCC
R_{free} test set	1465 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 72.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3863	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATE

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	0.39	0/1947	0.58	1/2634 (0.0%)
1	B	0.36	0/1935	0.58	0/2618
All	All	0.37	0/3882	0.58	1/5252 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	LEU	CA-CB-CG	7.37	132.25	115.30

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	1901	0	1898	73	0
1	B	1889	0	1894	106	6
2	A	20	0	30	0	0
2	B	20	0	30	0	0
3	A	18	0	0	0	0
3	B	15	0	0	0	0
All	All	3863	0	3852	175	6

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 23.

All (175) 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:B:271:LEU:HD23	1:B:302:LEU:HD23	1.49	0.93
1:A:266:GLU:HB2	1:A:267:PRO:HD3	1.56	0.88
1:A:138:LEU:HD21	1:A:178:MET:HG2	1.60	0.84
1:A:117:ASN:ND2	1:A:120:GLN:H	1.75	0.83
1:A:117:ASN:HD22	1:A:117:ASN:C	1.83	0.81
1:A:127:LEU:HB3	1:A:270:VAL:HG11	1.65	0.77
1:A:221:CYS:HG	1:B:221:CYS:HG	1.07	0.77
1:A:127:LEU:HB3	1:A:270:VAL:CG1	2.18	0.74
1:A:114:LEU:O	1:A:115:GLN:HB2	1.88	0.72
1:A:148:PRO:HD2	1:A:151:LEU:HD22	1.73	0.71
1:A:216:LEU:HD22	1:A:227:PHE:CD2	2.26	0.71
1:B:236:MET:HE3	1:B:249:LEU:HB3	1.74	0.69
1:A:215:SER:O	1:A:218:THR:HB	1.93	0.68
1:A:117:ASN:HD21	1:A:120:GLN:H	1.41	0.68
1:B:287:GLN:C	1:B:289:GLU:H	1.97	0.67
1:B:120:GLN:HG2	1:B:121:LYS:NZ	2.09	0.67
1:A:117:ASN:HD21	1:A:120:GLN:HG3	1.59	0.66
1:B:197:MET:O	1:B:201:ILE:HG12	1.96	0.66
1:A:282:ARG:HH11	1:A:282:ARG:HG2	1.61	0.66
1:B:329:LEU:O	1:B:332:ILE:HG13	1.96	0.66
1:A:306:ILE:HD13	1:A:318:LEU:HD13	1.78	0.65
1:B:124:VAL:O	1:B:128:LEU:HD23	1.97	0.64
1:A:135:VAL:O	1:A:138:LEU:HB3	1.96	0.64
1:B:280:PRO:HD3	1:B:291:ILE:HG22	1.79	0.64
1:B:251:SER:HB3	1:B:332:ILE:HG21	1.81	0.63
1:B:267:PRO:O	1:B:271:LEU:HB2	1.99	0.62
1:A:201:ILE:O	1:A:205:LYS:HB2	2.00	0.62
1:A:216:LEU:HD22	1:A:227:PHE:HD2	1.65	0.62
1:B:196:THR:HG23	1:B:199:ASP:HB2	1.81	0.61
1:A:231:PRO:HB3	1:B:155:HIS:ND1	2.15	0.61
1:B:127:LEU:HB3	1:B:270:VAL:CG1	2.30	0.61
1:A:117:ASN:ND2	1:A:120:GLN:HG3	2.17	0.60
1:B:226:ASN:OD1	1:B:235:LYS:HG2	2.01	0.60
1:A:191:LEU:HD21	1:A:294:LEU:HD22	1.85	0.59
1:A:197:MET:HE2	1:A:201:ILE:HG13	1.84	0.59
1:A:303:ASN:HD22	1:A:304:ASN:HD22	1.48	0.58
1:A:175:ASN:O	1:A:179:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:O	1:A:185:PHE:HB3	2.04	0.58
1:A:231:PRO:HB3	1:B:155:HIS:CE1	2.39	0.58
1:B:301:ILE:HD12	1:B:301:ILE:N	2.19	0.57
1:B:138:LEU:CD1	1:B:181:GLN:HG3	2.34	0.57
1:B:259:LEU:HD11	1:B:264:LEU:HD12	1.86	0.56
1:A:276:ALA:HB2	1:A:326:LEU:HD11	1.87	0.56
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.20	0.56
1:A:220:PHE:O	1:A:260:LYS:HE2	2.06	0.56
1:B:266:GLU:HB2	1:B:267:PRO:HD3	1.88	0.56
1:B:212:LEU:O	1:B:216:LEU:HB2	2.05	0.56
1:B:298:MET:HA	1:B:301:ILE:HB	1.88	0.55
1:B:138:LEU:HD11	1:B:178:MET:HA	1.89	0.55
1:B:127:LEU:HB3	1:B:270:VAL:HG12	1.89	0.55
1:A:181:GLN:HE22	1:A:184:LYS:NZ	2.05	0.55
1:B:271:LEU:CD2	1:B:302:LEU:HD23	2.32	0.55
1:B:271:LEU:HD23	1:B:302:LEU:CD2	2.29	0.54
1:B:120:GLN:HG2	1:B:121:LYS:HZ3	1.71	0.54
1:B:291:ILE:C	1:B:293:GLN:H	2.10	0.54
1:B:120:GLN:C	1:B:122:GLU:H	2.09	0.54
1:A:266:GLU:HB2	1:A:267:PRO:CD	2.34	0.53
1:A:303:ASN:HD22	1:A:304:ASN:ND2	2.06	0.53
1:B:223:GLN:C	1:B:223:GLN:HE21	2.12	0.53
1:B:209:VAL:HB	1:B:333:ASN:ND2	2.24	0.52
1:A:199:ASP:O	1:A:203:LEU:HG	2.09	0.52
1:A:306:ILE:CD1	1:A:318:LEU:HD13	2.39	0.52
1:B:141:GLN:HE21	1:B:144:GLN:HG3	1.74	0.52
1:B:120:GLN:C	1:B:122:GLU:N	2.62	0.52
1:B:334:ASN:O	1:B:335:ALA:C	2.47	0.52
1:A:220:PHE:CZ	1:A:225:GLU:HA	2.44	0.51
1:B:141:GLN:NE2	1:B:144:GLN:HG3	2.26	0.51
1:A:186:THR:HG21	1:A:204:LEU:HD21	1.92	0.51
1:B:121:LYS:HZ3	1:B:121:LYS:HA	1.75	0.50
1:A:179:VAL:O	1:A:183:ILE:HG13	2.11	0.50
1:B:322:LEU:O	1:B:325:LEU:HB2	2.11	0.50
1:A:148:PRO:HD2	1:A:151:LEU:CD2	2.42	0.49
1:B:129:GLY:O	1:B:133:ARG:HG3	2.12	0.49
1:B:121:LYS:HZ3	1:B:121:LYS:CA	2.25	0.49
1:B:332:ILE:C	1:B:332:ILE:HD12	2.32	0.49
1:A:285:VAL:HG22	1:A:288:ARG:NH2	2.27	0.49
1:B:236:MET:CE	1:B:249:LEU:HB3	2.41	0.49
1:B:266:GLU:O	1:B:270:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:HA	1:A:118:GLN:NE2	2.28	0.49
1:B:231:PRO:HG2	1:B:232:LEU:HD13	1.95	0.49
1:B:287:GLN:C	1:B:289:GLU:N	2.66	0.49
1:A:117:ASN:ND2	1:A:117:ASN:C	2.57	0.48
1:B:150:TYR:OH	1:B:167:LEU:HD22	2.12	0.48
1:A:201:ILE:HG22	1:A:205:LYS:HE3	1.96	0.48
1:B:312:ARG:HH12	1:B:313:LEU:HD21	1.78	0.48
1:B:299:ALA:HB1	1:B:319:TYR:OH	2.14	0.48
1:B:312:ARG:NH1	1:B:313:LEU:HD21	2.29	0.47
1:B:178:MET:CE	1:B:212:LEU:HG	2.44	0.47
1:B:318:LEU:O	1:B:321:LYS:N	2.47	0.47
1:B:138:LEU:HD12	1:B:181:GLN:HG3	1.96	0.47
1:A:123:LEU:HD23	1:A:301:ILE:CD1	2.45	0.47
1:B:216:LEU:HD22	1:B:227:PHE:CD2	2.50	0.47
1:B:125:GLN:HA	1:B:125:GLN:NE2	2.30	0.47
1:B:351:PRO:O	1:B:352:LEU:HD23	2.15	0.46
1:B:259:LEU:HD11	1:B:264:LEU:CD1	2.45	0.46
1:A:278:PHE:O	1:A:295:GLN:HB2	2.15	0.46
1:B:120:GLN:O	1:B:123:LEU:HB3	2.15	0.46
1:B:297:GLU:C	1:B:301:ILE:HD13	2.36	0.46
1:B:310:GLN:NE2	1:B:311:SER:N	2.64	0.46
1:B:298:MET:HB2	1:B:298:MET:HE3	1.82	0.45
1:A:265:GLN:O	1:A:266:GLU:C	2.54	0.45
1:B:317:PHE:O	1:B:321:LYS:HG3	2.16	0.45
1:B:164:VAL:HG23	1:B:165:LEU:N	2.32	0.45
1:B:190:PRO:HG2	1:B:191:LEU:H	1.80	0.45
1:B:323:MET:HE2	1:B:323:MET:HA	1.99	0.45
1:B:296:GLU:C	1:B:298:MET:H	2.19	0.45
1:A:118:GLN:HE21	1:A:118:GLN:CA	2.29	0.45
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.82	0.45
1:B:121:LYS:NZ	1:B:121:LYS:HA	2.31	0.45
1:B:147:PRO:HB3	1:B:170:HIS:CE1	2.52	0.44
1:B:281:ASP:HB3	1:B:330:ARG:HH22	1.82	0.44
1:B:213:HIS:CE1	1:B:252:ILE:HD12	2.52	0.44
1:A:141:GLN:HB2	1:A:177:PHE:HE1	1.82	0.44
1:B:316:ARG:O	1:B:317:PHE:HB2	2.17	0.44
1:A:178:MET:O	1:A:182:ILE:HG13	2.18	0.44
1:B:127:LEU:HB3	1:B:270:VAL:HG11	1.99	0.44
1:A:253:LEU:O	1:A:257:LYS:HG3	2.17	0.44
1:B:334:ASN:O	1:B:336:TYR:N	2.50	0.44
1:B:179:VAL:O	1:B:183:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLY:HA3	1:A:163:PRO:HD2	1.85	0.43
1:A:165:LEU:HB3	1:A:166:PRO:CD	2.49	0.43
1:A:237:GLU:H	1:A:237:GLU:CD	2.21	0.43
1:A:293:GLN:O	1:A:297:GLU:HG3	2.17	0.43
1:B:337:SER:HA	1:B:340:LEU:HD13	1.99	0.43
1:A:114:LEU:O	1:A:115:GLN:CB	2.62	0.43
1:A:263:HIS:NE2	1:B:263:HIS:CE1	2.87	0.43
1:B:220:PHE:O	1:B:260:LYS:HE2	2.18	0.43
1:A:297:GLU:O	1:A:301:ILE:HG13	2.19	0.43
1:B:120:GLN:OE1	1:B:121:LYS:HE2	2.19	0.43
1:B:164:VAL:HG12	1:B:241:HIS:NE2	2.33	0.43
1:B:302:LEU:HD11	1:B:322:LEU:HD23	2.01	0.43
1:A:116:LEU:HA	1:A:120:GLN:OE1	2.19	0.42
1:A:210:GLU:HA	1:A:329:LEU:HD21	2.00	0.42
1:B:246:TYR:O	1:B:247:GLU:C	2.58	0.42
1:B:301:ILE:N	1:B:301:ILE:CD1	2.82	0.42
1:A:148:PRO:O	1:A:151:LEU:HB2	2.20	0.42
1:B:318:LEU:HD22	1:B:322:LEU:HD13	2.01	0.42
1:B:120:GLN:CD	1:B:121:LYS:HE2	2.40	0.42
1:B:207:ALA:O	1:B:208:ALA:C	2.58	0.42
1:A:328:ASP:O	1:A:332:ILE:HG13	2.20	0.42
1:B:318:LEU:O	1:B:319:TYR:C	2.57	0.42
1:A:136:GLY:N	1:A:137:PRO:CD	2.83	0.41
1:B:302:LEU:O	1:B:306:ILE:HG13	2.20	0.41
1:B:324:GLY:O	1:B:328:ASP:OD1	2.38	0.41
1:B:339:GLU:C	1:B:341:GLN:N	2.73	0.41
1:B:353:LEU:C	1:B:355:GLU:H	2.23	0.41
1:A:257:LYS:HE2	1:A:257:LYS:HB3	1.87	0.41
1:B:178:MET:HE2	1:B:212:LEU:HG	2.01	0.41
1:B:210:GLU:HB3	1:B:329:LEU:HD23	2.03	0.41
1:B:280:PRO:HG3	1:B:292:ASP:HA	2.02	0.41
1:A:117:ASN:HD22	1:A:120:GLN:H	1.63	0.41
1:A:121:LYS:O	1:A:125:GLN:HG2	2.20	0.41
1:B:210:GLU:HG3	1:B:333:ASN:HD22	1.85	0.41
1:B:307:MET:C	1:B:309:GLN:N	2.73	0.41
1:A:118:GLN:HE21	1:A:118:GLN:HA	1.84	0.41
1:B:265:GLN:OE1	1:B:312:ARG:CZ	2.69	0.41
1:A:252:ILE:HD13	1:A:252:ILE:HA	1.91	0.41
1:B:272:MET:CE	1:B:326:LEU:HD13	2.50	0.41
1:B:332:ILE:HD12	1:B:333:ASN:N	2.36	0.41
1:A:268:GLU:OE2	1:A:305:HIS:HE1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLY:O	1:A:327:ALA:HB3	2.21	0.41
1:B:229:CYS:O	1:B:232:LEU:HB2	2.21	0.41
1:B:353:LEU:C	1:B:355:GLU:N	2.74	0.41
1:A:127:LEU:HB3	1:A:270:VAL:HG12	2.00	0.41
1:B:121:LYS:HZ3	1:B:121:LYS:N	2.19	0.41
1:B:241:HIS:C	1:B:243:GLY:N	2.74	0.41
1:B:210:GLU:OE1	1:B:330:ARG:HA	2.21	0.40
1:B:351:PRO:C	1:B:352:LEU:HD23	2.42	0.40
1:A:199:ASP:OD1	1:A:287:GLN:HG2	2.20	0.40
1:B:124:VAL:HG12	1:B:124:VAL:O	2.21	0.40
1:B:180:GLN:O	1:B:184:LYS:HG3	2.21	0.40
1:B:287:GLN:O	1:B:289:GLU:N	2.53	0.40
1:A:118:GLN:HG3	1:A:122:GLU:OE2	2.22	0.40
1:A:197:MET:CE	1:A:201:ILE:HG13	2.51	0.40
1:A:282:ARG:O	1:A:285:VAL:HG13	2.22	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLN:OE1	1:B:341:GLN:NE2[4_566]	0.79	1.41
1:B:341:GLN:CD	1:B:341:GLN:NE2[4_566]	0.83	1.37
1:B:341:GLN:CD	1:B:341:GLN:CD[4_566]	1.43	0.77
1:B:341:GLN:NE2	1:B:341:GLN:NE2[4_566]	1.65	0.55
1:B:341:GLN:CD	1:B:341:GLN:OE1[4_566]	2.06	0.14
1:B:341:GLN:CG	1:B:341:GLN:NE2[4_566]	2.18	0.02

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	230/256 (90%)	215 (94%)	13 (6%)	2 (1%)	17 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	228/256 (89%)	198 (87%)	24 (10%)	6 (3%)	5 20
All	All	458/512 (90%)	413 (90%)	37 (8%)	8 (2%)	9 31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	B	246	TYR
1	B	288	ARG
1	B	318	LEU
1	B	335	ALA
1	B	342	ARG
1	B	319	TYR
1	A	266	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	209/229 (91%)	198 (95%)	11 (5%)	22 54
1	B	208/229 (91%)	189 (91%)	19 (9%)	9 28
All	All	417/458 (91%)	387 (93%)	30 (7%)	14 39

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	151	LEU
1	A	165	LEU
1	A	216	LEU
1	A	222	LEU
1	A	232	LEU
1	A	249	LEU
1	A	253	LEU

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Mol	Chain	Res	Type
1	A	289	GLU
1	A	302	LEU
1	A	318	LEU
1	B	121	LYS
1	B	122	GLU
1	B	128	LEU
1	B	165	LEU
1	B	188	ASP
1	B	205	LYS
1	B	216	LEU
1	B	223	GLN
1	B	232	LEU
1	B	247	GLU
1	B	268	GLU
1	B	271	LEU
1	B	275	THR
1	B	302	LEU
1	B	303	ASN
1	B	315	SER
1	B	326	LEU
1	B	328	ASP
1	B	353	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	118	GLN
1	A	125	GLN
1	A	175	ASN
1	A	181	GLN
1	A	200	GLN
1	A	217	ASN
1	A	245	GLN
1	A	258	ASN
1	A	265	GLN
1	A	293	GLN
1	A	304	ASN
1	A	305	HIS
1	A	309	GLN
1	A	341	GLN
1	B	125	GLN

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Mol	Chain	Res	Type
1	B	131	HIS
1	B	141	GLN
1	B	144	GLN
1	B	159	GLN
1	B	175	ASN
1	B	180	GLN
1	B	181	GLN
1	B	217	ASN
1	B	223	GLN
1	B	263	HIS
1	B	303	ASN
1	B	310	GLN
1	B	333	ASN
1	B	334	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
2	ATE	B	600	-	21,23,23	1.41	3 (14%)	32,37,37	2.55	14 (43%)
2	ATE	A	500	-	21,23,23	1.32	3 (14%)	32,37,37	2.56	14 (43%)

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	ATE	B	600	-	-	-	0/4/4/4
2	ATE	A	500	-	-	-	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ATE	C8-C9	3.06	1.59	1.53
2	A	500	ATE	C8-C9	2.86	1.59	1.53
2	B	600	ATE	C10-C5	2.39	1.59	1.55
2	B	600	ATE	C19-C10	2.33	1.58	1.54
2	A	500	ATE	C10-C5	2.10	1.58	1.55
2	A	500	ATE	C19-C10	2.05	1.57	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	ATE	C4-C3-C2	7.56	119.58	110.55
2	B	600	ATE	C4-C3-C2	7.35	119.33	110.55
2	B	600	ATE	C19-C10-C9	-4.27	105.30	111.18
2	A	500	ATE	C19-C10-C9	-4.20	105.40	111.18
2	B	600	ATE	C7-C8-C9	3.73	115.11	110.49
2	A	500	ATE	C10-C9-C8	-3.66	108.57	112.42
2	A	500	ATE	C7-C8-C9	3.62	114.98	110.49
2	B	600	ATE	C18-C13-C12	-3.56	106.95	111.12
2	B	600	ATE	C10-C9-C8	-3.47	108.78	112.42
2	A	500	ATE	O1-C3-C4	-3.47	102.95	109.85
2	B	600	ATE	O1-C3-C4	-3.42	103.05	109.85
2	A	500	ATE	C18-C13-C12	-3.34	107.20	111.12
2	A	500	ATE	C9-C10-C5	3.30	113.22	108.58
2	B	600	ATE	C9-C10-C5	3.27	113.17	108.58
2	B	600	ATE	C14-C15-C16	-3.21	97.30	104.10
2	A	500	ATE	C14-C15-C16	-3.16	97.41	104.10
2	A	500	ATE	C12-C13-C17	2.80	124.13	115.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	ATE	C12-C13-C14	2.78	113.40	108.98
2	B	600	ATE	C12-C13-C17	2.75	123.95	115.03
2	A	500	ATE	C4-C5-C10	2.57	115.39	112.66
2	B	600	ATE	C4-C5-C10	2.50	115.32	112.66
2	A	500	ATE	C12-C13-C14	2.39	112.78	108.98
2	B	600	ATE	C15-C14-C13	2.32	105.79	104.05
2	A	500	ATE	C15-C14-C13	2.30	105.77	104.05
2	B	600	ATE	C2-C1-C10	2.25	116.64	112.78
2	B	600	ATE	C13-C14-C8	2.20	115.47	113.11
2	A	500	ATE	C13-C14-C8	2.19	115.46	113.11
2	A	500	ATE	C2-C1-C10	2.19	116.54	112.78

There are no chirality outliers.

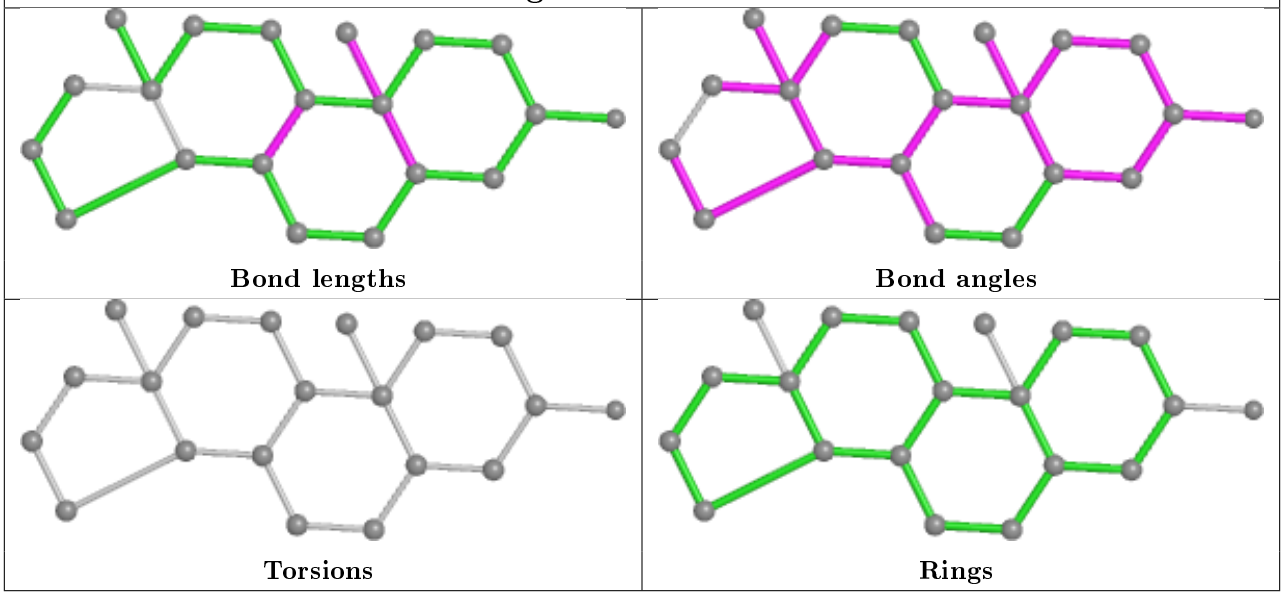
There are no torsion outliers.

There are no ring outliers.

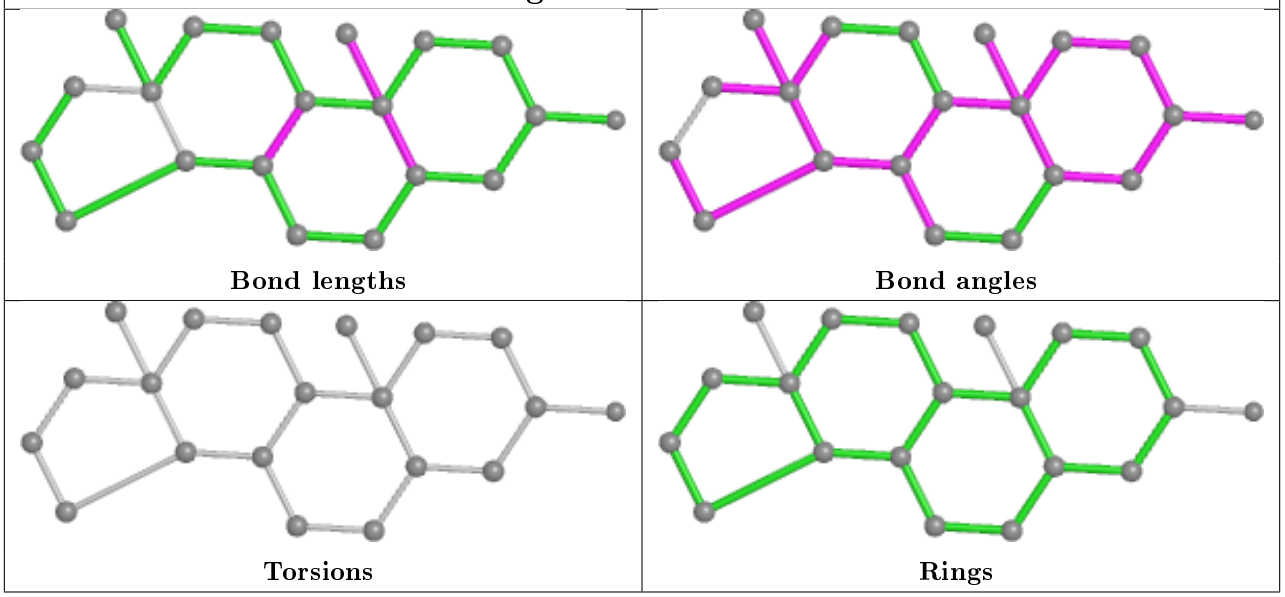
No monomer is involved in short contacts.

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 ATE B 600



Ligand ATE A 500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	232/256 (90%)	-0.10	8 (3%) 45 40	18, 30, 53, 67	0
1	B	232/256 (90%)	0.40	25 (10%) 5 4	21, 50, 93, 112	0
All	All	464/512 (90%)	0.15	33 (7%) 16 12	18, 38, 81, 112	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	GLN	6.9
1	B	293	GLN	6.3
1	B	286	THR	5.4
1	B	357	CYS	5.3
1	A	198	GLU	4.8
1	B	121	LYS	4.1
1	B	304	ASN	4.0
1	B	338	TYR	4.0
1	B	133	ARG	3.7
1	A	197	MET	3.6
1	B	336	TYR	3.6
1	B	310	GLN	3.6
1	A	334	ASN	3.6
1	B	285	VAL	3.1
1	A	289	GLU	3.0
1	B	335	ALA	3.0
1	A	290	GLU	3.0
1	B	283	PRO	2.8
1	B	280	PRO	2.8
1	B	337	SER	2.6
1	B	291	ILE	2.5
1	A	246	TYR	2.5
1	B	311	SER	2.5
1	B	289	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	281	ASP	2.4
1	B	334	ASN	2.2
1	B	331	SER	2.1
1	B	308	GLU	2.1
1	B	288	ARG	2.1
1	B	299	ALA	2.0
1	A	118	GLN	2.0
1	B	196	THR	2.0
1	B	352	LEU	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 carbohydrates in this entry.

6.4 Ligands (i)

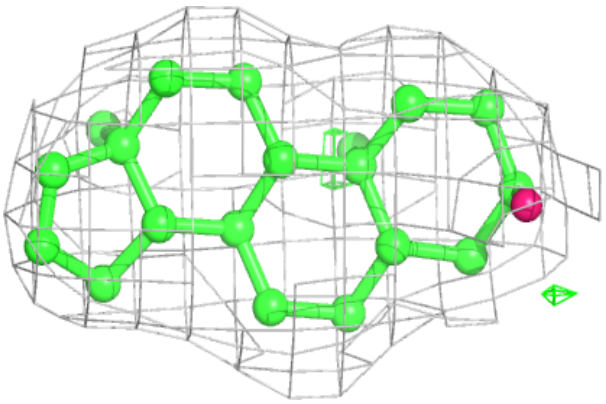
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

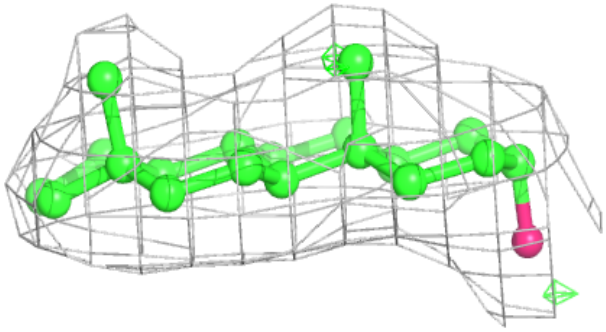
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ATE	B	600	20/20	0.92	0.38	52,54,59,59	0
2	ATE	A	500	20/20	0.95	0.33	24,31,41,44	0

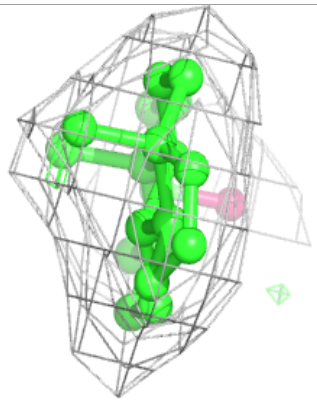
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATE B 600:

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

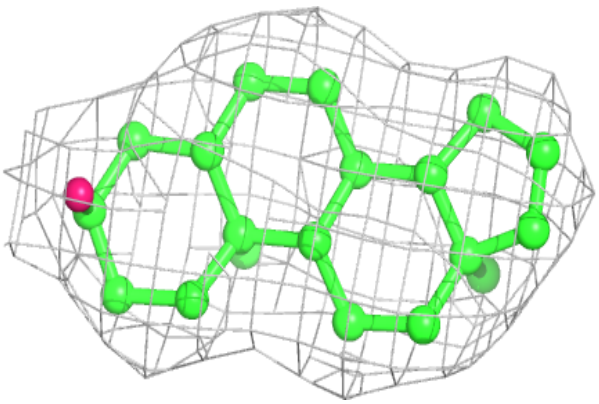


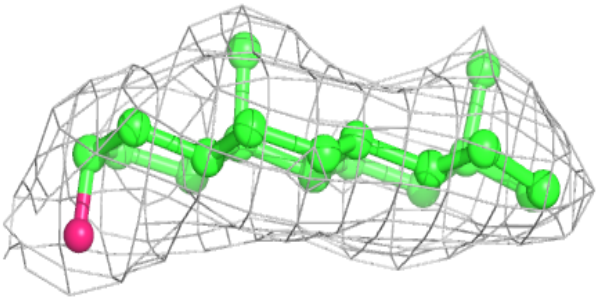


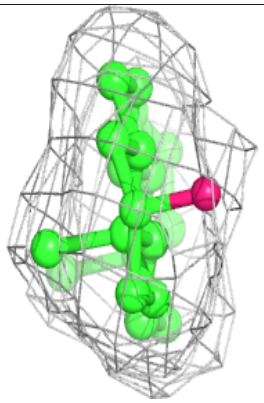


Electron density around ATE A 500:

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







6.5 Other polymers (i)

There are no such residues in this entry.