Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 06:59 PM EDT

PDB ID	:	3OLL
Title	:	Crystal structure of phosphorylated estrogen receptor beta ligand binding domain
Authors	:	Moecklinghoff, S.; Rose, R.; Ottmann, C.; Brunsveld, L.
Deposited on	:	2010-08-26
Resolution	:	1.50 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:

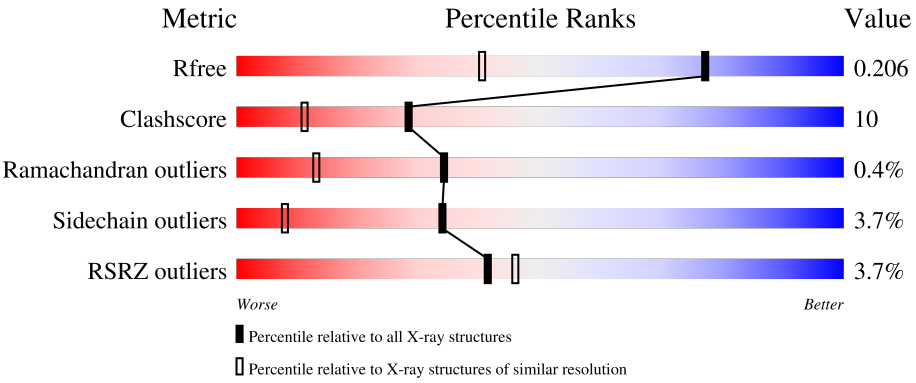
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	240	2% 80% 14%
1	B	240	3% 78% 16%
2	C	19	16% 32% 5% 16% 47%
2	D	19	16% 21% 11% 21% 47%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4521 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.

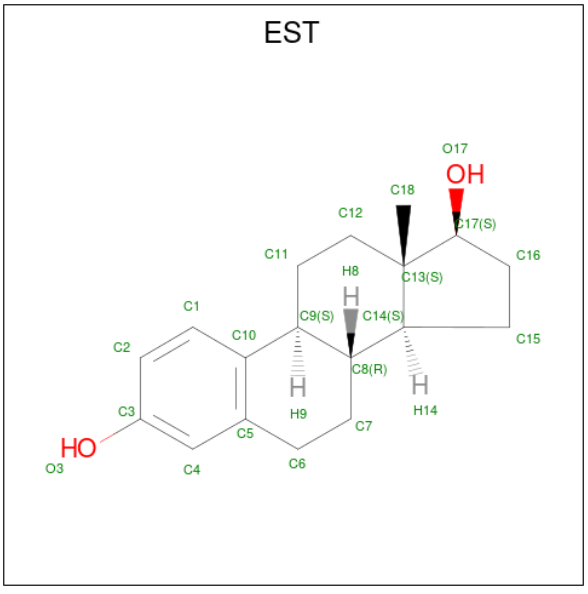
- Molecule 1 is a protein called Estrogen receptor beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	P	S	0	7	0
			1898	1212	318	345	1	22			
1	B	234	Total	C	N	O	P	S	0	6	0
			1889	1210	316	341	1	21			

- Molecule 2 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			92	59	22	11			
2	D	10	Total	C	N	O	0	0	0
			92	59	22	11			

- Molecule 3 is ESTRADIOL (three-letter code: EST) (formula: $C_{18}H_{24}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 18 2	0	0
3	B	1	Total C O 20 18 2	0	0

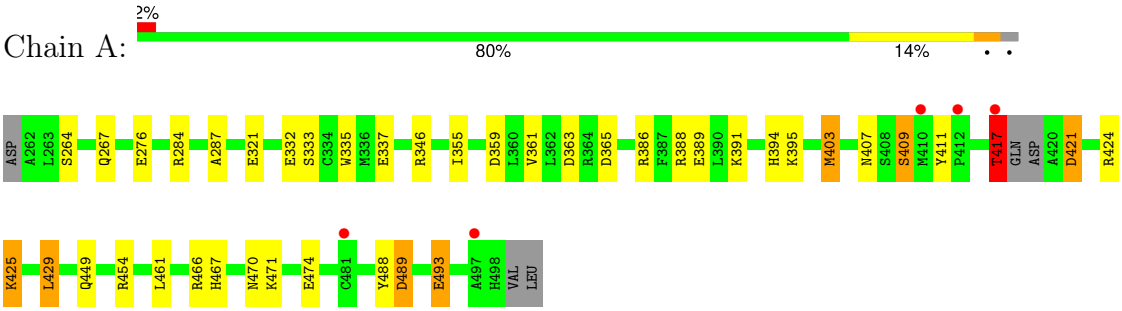
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	238	Total O 238 238	0	0
4	B	253	Total O 253 253	0	0
4	C	10	Total O 10 10	0	0
4	D	9	Total O 9 9	0	0

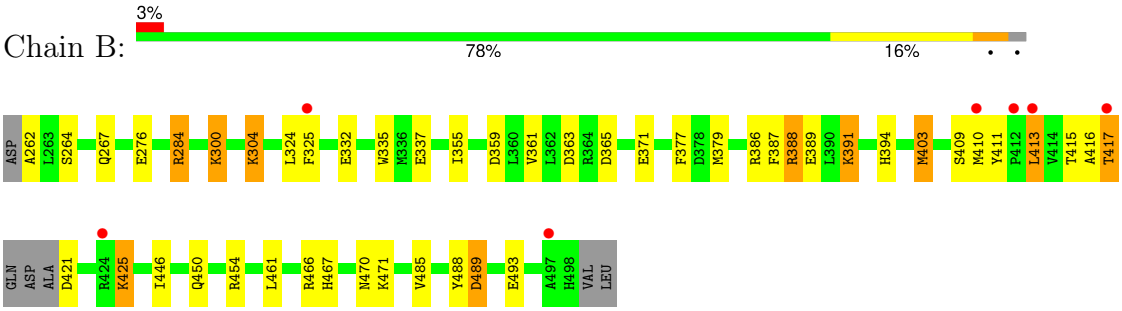
3 Residue-property plots (i)

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

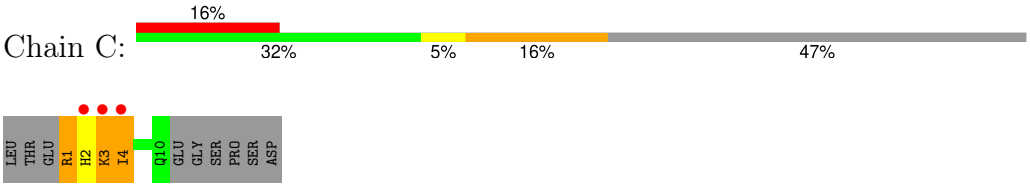
• Molecule 1: Estrogen receptor beta



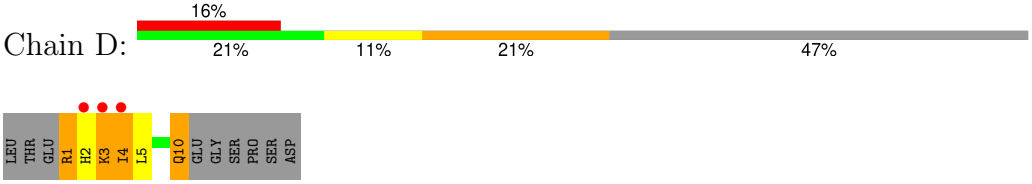
• Molecule 1: Estrogen receptor beta



• Molecule 2: Nuclear receptor coactivator 1



• Molecule 2: Nuclear receptor coactivator 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	71.86Å 71.86Å 113.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.16 – 1.50 19.16 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.16-1.50) 99.9 (19.16-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.208 0.173 , 0.206	Depositor DCC
R_{free} test set	5230 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l 0.488 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4521	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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 (i)

5.1 Standard geometry (i)

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

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	1.70	17/1914 (0.9%)	1.18	16/2584 (0.6%)
1	B	1.74	21/1906 (1.1%)	1.37	21/2573 (0.8%)
2	C	1.71	1/93 (1.1%)	1.48	1/122 (0.8%)
2	D	1.92	3/93 (3.2%)	1.59	1/122 (0.8%)
All	All	1.72	42/4006 (1.0%)	1.29	39/5401 (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	B	0	1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	ARG	CD-NE	-10.94	1.27	1.46
1	B	304	LYS	CG-CD	-8.32	1.24	1.52
1	B	337	GLU	CD-OE1	8.27	1.34	1.25
1	A	337	GLU	CD-OE1	8.16	1.34	1.25
1	A	276	GLU	CG-CD	7.73	1.63	1.51
1	B	371	GLU	CG-CD	7.68	1.63	1.51
1	B	304	LYS	CB-CG	-7.48	1.32	1.52
1	B	389	GLU	CB-CG	-7.45	1.38	1.52
1	B	411	TYR	CE1-CZ	-7.36	1.28	1.38
1	B	276	GLU	CG-CD	7.35	1.62	1.51
1	B	276	GLU	CD-OE1	-6.98	1.18	1.25
1	A	389	GLU	CB-CG	-6.56	1.39	1.52
1	A	417	THR	CA-CB	-6.46	1.36	1.53
1	A	276	GLU	CD-OE1	-6.07	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	429	LEU	CG-CD1	-6.05	1.29	1.51
2	D	4	ILE	CA-C	6.02	1.68	1.52
1	A	389	GLU	CD-OE1	5.93	1.32	1.25
1	A	474	GLU	CG-CD	5.91	1.60	1.51
1	A	407	ASN	C-O	-5.89	1.12	1.23
1	B	417	THR	C-O	5.87	1.34	1.23
2	D	10	GLN	CB-CG	5.80	1.68	1.52
1	B	389	GLU	CG-CD	5.63	1.60	1.51
1	A	287	ALA	CA-CB	-5.61	1.40	1.52
1	A	335	TRP	CE3-CZ3	5.58	1.48	1.38
1	B	284	ARG	NE-CZ	5.58	1.40	1.33
1	B	335	TRP	CE3-CZ3	5.53	1.47	1.38
1	B	388	ARG	CD-NE	-5.49	1.37	1.46
1	A	411	TYR	CE2-CZ	-5.42	1.31	1.38
1	A	389	GLU	CG-CD	5.39	1.60	1.51
2	C	4	ILE	CA-C	5.32	1.66	1.52
1	A	388	ARG	CD-NE	-5.31	1.37	1.46
2	D	10	GLN	CG-CD	5.21	1.63	1.51
1	B	371	GLU	CB-CG	-5.16	1.42	1.52
1	A	333	SER	CB-OG	5.15	1.49	1.42
1	B	410	MET	CG-SD	-5.15	1.67	1.81
1	B	387	PHE	CB-CG	5.13	1.60	1.51
1	A	493	GLU	CB-CG	5.08	1.61	1.52
1	B	377	PHE	CE1-CZ	5.06	1.47	1.37
1	A	267	GLN	CG-CD	5.04	1.62	1.51
1	B	267	GLN	C-O	5.01	1.32	1.23
1	B	264	SER	CB-OG	-5.00	1.35	1.42
1	B	485	VAL	CA-CB	5.00	1.65	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	284	ARG	NE-CZ-NH2	25.38	132.99	120.30
1	B	388	ARG	NE-CZ-NH1	14.76	127.68	120.30
1	B	388	ARG	NE-CZ-NH2	-14.67	112.97	120.30
1	B	284	ARG	NE-CZ-NH1	-14.13	113.23	120.30
1	B	284	ARG	CD-NE-CZ	14.04	143.26	123.60
1	B	454	ARG	NE-CZ-NH2	12.77	126.69	120.30
1	A	388	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	A	284	ARG	NE-CZ-NH2	10.72	125.66	120.30
1	A	388	ARG	NE-CZ-NH1	10.59	125.60	120.30
1	A	454	ARG	NE-CZ-NH2	10.34	125.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	417	THR	CB-CA-C	-9.12	86.97	111.60
1	B	489	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	B	389	GLU	CA-CB-CG	7.23	129.31	113.40
1	B	416	ALA	C-N-CA	7.19	139.67	121.70
1	A	363	ASP	CB-CG-OD1	7.00	124.59	118.30
1	B	454	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	B	284	ARG	CG-CD-NE	-6.42	98.32	111.80
1	B	409	SER	CB-CA-C	-6.40	97.94	110.10
1	A	403	MET	CG-SD-CE	-6.31	90.11	100.20
1	B	388	ARG	CD-NE-CZ	6.20	132.28	123.60
1	A	417	THR	CB-CA-C	-6.12	95.07	111.60
1	B	363	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	403	MET	CG-SD-CE	-6.10	90.44	100.20
1	B	264	SER	N-CA-CB	-5.89	101.66	110.50
1	A	489	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	300	LYS	CD-CE-NZ	5.72	124.86	111.70
1	B	417	THR	N-CA-C	5.71	126.43	111.00
1	A	409	SER	CB-CA-C	-5.62	99.42	110.10
1	A	407	ASN	C-N-CA	-5.60	107.69	121.70
1	A	365	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	421	ASP	CB-CG-OD1	5.58	123.32	118.30
2	C	3	LYS	N-CA-C	5.43	125.66	111.00
1	A	365	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	B	284	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
2	D	3	LYS	N-CA-C	5.30	125.32	111.00
1	B	365	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	489	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	346	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	417	THR	CA-CB-OG1	-5.05	98.40	109.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	388	ARG	Sidechain

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	1898	0	1954	26	0
1	B	1889	0	1948	42	1
2	C	92	0	107	17	0
2	D	92	0	107	17	0
3	A	20	0	24	0	0
3	B	20	0	24	0	0
4	A	238	0	0	9	0
4	B	253	0	0	13	1
4	C	10	0	0	4	0
4	D	9	0	0	0	0
All	All	4521	0	4164	80	1

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 10.

All (80) 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:332:GLU:OE2	2:C:2:HIS:NE2	1.79	1.14
1:B:493:GLU:OE2	2:D:4:ILE:HB	1.65	0.97
1:B:332:GLU:OE2	2:D:2:HIS:CD2	2.25	0.90
1:A:332:GLU:OE2	2:C:2:HIS:CD2	2.24	0.90
1:A:425:LYS:HD3	4:A:560:HOH:O	1.83	0.77
1:B:493:GLU:OE2	2:D:4:ILE:CB	2.33	0.76
1:A:424:ARG:HG3	4:A:583:HOH:O	1.87	0.74
1:A:417:THR:O	1:A:417:THR:CG2	2.29	0.73
1:B:425:LYS:HD3	4:B:554:HOH:O	1.90	0.72
1:B:421:ASP:N	4:B:623:HOH:O	2.25	0.70
1:B:332:GLU:OE2	2:D:2:HIS:NE2	2.26	0.69
1:A:417:THR:O	1:A:417:THR:HG23	1.92	0.69
1:B:262:ALA:N	4:B:584:HOH:O	2.26	0.68
1:B:284:ARG:CD	4:B:571:HOH:O	2.40	0.68
1:B:325[B]:PHE:CE2	1:B:413:LEU:HD13	2.31	0.66
2:C:3:LYS:CE	4:C:288:HOH:O	2.43	0.66
1:A:493:GLU:OE2	2:C:4:ILE:HB	1.95	0.65
1:B:493:GLU:OE2	2:D:4:ILE:N	2.29	0.65
1:B:284:ARG:HD2	4:B:26:HOH:O	1.96	0.64
2:C:1:ARG:N	4:C:288:HOH:O	2.31	0.64
1:B:284:ARG:HD2	4:B:571:HOH:O	1.98	0.64
1:B:324:LEU:HD21	2:D:10:GLN:NE2	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:ARG:HG2	2:D:1:ARG:HH11	1.62	0.63
2:C:3:LYS:HE3	4:C:288:HOH:O	2.01	0.60
1:B:284:ARG:HD3	4:B:571:HOH:O	2.01	0.60
1:A:493:GLU:OE2	2:C:4:ILE:CB	2.50	0.60
1:B:324:LEU:CD2	2:D:10:GLN:NE2	2.64	0.60
2:C:1:ARG:HH11	2:C:1:ARG:HG2	1.66	0.59
1:A:425:LYS:CG	4:A:560:HOH:O	2.51	0.58
1:A:470:ASN:HB3	1:B:470:ASN:ND2	2.19	0.57
1:A:493:GLU:OE2	2:C:4:ILE:N	2.32	0.57
1:A:425:LYS:O	1:A:429:LEU:HD13	2.05	0.56
1:B:379:MET:HE1	1:B:467:HIS:ND1	2.20	0.56
2:C:1:ARG:N	2:C:3:LYS:HG3	2.20	0.56
1:B:355:ILE:HD13	1:B:361:VAL:HG13	1.88	0.56
1:A:493:GLU:OE2	2:C:4:ILE:CG1	2.54	0.55
1:A:467:HIS:HD2	1:B:466:ARG:HD2	1.72	0.55
1:B:379:MET:CE	1:B:467:HIS:ND1	2.69	0.55
1:A:355:ILE:HD13	1:A:361:VAL:HG13	1.90	0.54
1:B:324:LEU:CD2	2:D:10:GLN:HE21	2.19	0.54
1:A:466:ARG:HD2	1:B:467:HIS:HD2	1.73	0.53
1:B:325[B]:PHE:CE2	1:B:413:LEU:CD1	2.91	0.53
2:C:1:ARG:HH11	2:C:1:ARG:CG	2.21	0.53
1:B:325[B]:PHE:HE2	1:B:413:LEU:CD1	2.22	0.52
1:B:425:LYS:CG	4:B:554:HOH:O	2.57	0.52
2:D:1:ARG:HH11	2:D:1:ARG:CG	2.21	0.52
1:B:386:ARG:HG2	1:B:461:LEU:HD21	1.91	0.51
1:B:324:LEU:HD22	2:D:10:GLN:HE21	1.75	0.51
2:C:1:ARG:H2	2:C:3:LYS:HG3	1.76	0.50
1:A:493:GLU:OE2	2:C:4:ILE:HG13	2.12	0.49
2:D:1:ARG:N	2:D:3:LYS:HG3	2.27	0.49
1:A:425:LYS:CD	4:A:560:HOH:O	2.50	0.48
1:B:415:THR:OG1	1:B:417:THR:HG23	2.13	0.48
1:B:493:GLU:OE2	2:D:4:ILE:CG1	2.61	0.48
1:A:471:LYS:HD2	4:A:547:HOH:O	2.14	0.47
1:B:471:LYS:HD2	4:B:603:HOH:O	2.15	0.47
2:D:1:ARG:CG	2:D:1:ARG:NH1	2.76	0.47
2:D:1:ARG:HD2	2:D:2:HIS:CE1	2.50	0.47
1:A:394:HIS:HE1	4:A:158:HOH:O	1.97	0.46
1:B:493:GLU:CD	2:D:4:ILE:HB	2.34	0.46
2:C:1:ARG:CG	2:C:1:ARG:NH1	2.77	0.46
1:B:325[B]:PHE:HE2	1:B:413:LEU:HD11	1.81	0.45
1:B:394:HIS:HE1	4:B:598:HOH:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:SER:HB2	4:A:598:HOH:O	2.16	0.45
1:B:493:GLU:CD	2:D:4:ILE:H	2.17	0.44
1:B:325[B]:PHE:CZ	1:B:413:LEU:HD13	2.53	0.44
1:B:425:LYS:HG2	4:B:554:HOH:O	2.16	0.44
1:A:471:LYS:CE	4:A:593:HOH:O	2.66	0.43
1:B:300:LYS:HE2	1:B:300:LYS:HB2	1.69	0.43
1:A:425:LYS:HG2	4:A:560:HOH:O	2.15	0.42
1:A:386:ARG:HG2	1:A:461:LEU:HD21	2.01	0.42
1:B:403:MET:HB3	1:B:403:MET:HE3	1.71	0.41
1:B:471:LYS:CE	4:B:579:HOH:O	2.68	0.41
1:A:403:MET:HE3	1:A:403:MET:HB3	1.85	0.41
2:C:1:ARG:HD2	2:C:2:HIS:CE1	2.56	0.41
1:B:446:ILE:HD12	1:B:450:GLN:HB3	2.02	0.41
1:B:391:LYS:HD3	4:B:172:HOH:O	2.21	0.40
2:C:3:LYS:HE2	4:C:288:HOH:O	2.13	0.40
1:B:421:ASP:O	1:B:421:ASP:OD1	2.40	0.40
1:A:321[B]:GLU:HA	1:A:321[B]:GLU:OE2	2.21	0.40

All (1) 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:325[A]:PHE:CE1	4:B:501:HOH:O[2_565]	2.19	0.01

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	237/240 (99%)	231 (98%)	5 (2%)	1 (0%)	34	13
1	B	235/240 (98%)	228 (97%)	6 (3%)	1 (0%)	34	13
2	C	8/19 (42%)	7 (88%)	1 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	8/19 (42%)	7 (88%)	1 (12%)	0	100 100
All	All	488/518 (94%)	473 (97%)	13 (3%)	2 (0%)	34 13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP
1	B	489	ASP

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	216/214 (101%)	208 (96%)	8 (4%)	34 8
1	B	215/214 (100%)	210 (98%)	5 (2%)	50 20
2	C	10/18 (56%)	9 (90%)	1 (10%)	7 0
2	D	10/18 (56%)	8 (80%)	2 (20%)	1 0
All	All	451/464 (97%)	435 (96%)	16 (4%)	34 9

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	SER
1	A	359	ASP
1	A	391	LYS
1	A	395	LYS
1	A	417	THR
1	A	421	ASP
1	A	425	LYS
1	A	449	GLN
1	B	304	LYS
1	B	359	ASP
1	B	391	LYS
1	B	413	LEU

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Mol	Chain	Res	Type
1	B	425	LYS
2	C	1	ARG
2	D	1	ARG
2	D	5	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	HIS
1	A	407	ASN
1	A	449	GLN
1	A	450	GLN
1	A	467	HIS
1	A	496	ASN
1	A	498	HIS
1	B	394	HIS
1	B	407	ASN
1	B	450	GLN
1	B	470	ASN
1	B	498	HIS
2	D	2	HIS
2	D	10	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	PTR	A	488	1	15,16,17	1.82	2 (13%)	17,22,24	0.96	1 (5%)
1	PTR	B	488	1	15,16,17	1.69	4 (26%)	17,22,24	1.01	1 (5%)

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
1	PTR	A	488	1	-	0/10/11/13	0/1/1/1
1	PTR	B	488	1	-	0/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	488	PTR	OH-CZ	-5.12	1.29	1.40
1	B	488	PTR	OH-CZ	-4.32	1.31	1.40
1	A	488	PTR	CE2-CD2	3.06	1.43	1.38
1	B	488	PTR	CE2-CD2	2.48	1.42	1.38
1	B	488	PTR	P-OH	2.47	1.64	1.59
1	B	488	PTR	CD2-CG	2.20	1.43	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	488	PTR	OH-CZ-CE2	2.08	125.46	119.22
1	B	488	PTR	O3P-P-O2P	2.08	115.61	107.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EST	B	600	-	23,23,23	1.81	5 (21%)	36,36,36	1.27	6 (16%)
3	EST	A	600	-	23,23,23	2.07	9 (39%)	36,36,36	1.63	9 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EST	B	600	-	-	-	0/4/4/4
3	EST	A	600	-	-	-	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	EST	C5-C10	5.07	1.48	1.40
3	B	600	EST	C5-C10	5.06	1.48	1.40
3	A	600	EST	C2-C3	3.60	1.45	1.39
3	B	600	EST	C7-C8	3.13	1.58	1.53
3	A	600	EST	C6-C5	3.12	1.56	1.51
3	B	600	EST	C6-C5	2.81	1.55	1.51
3	A	600	EST	O3-C3	2.68	1.43	1.37
3	A	600	EST	C18-C13	2.63	1.58	1.54
3	A	600	EST	C7-C8	2.44	1.57	1.53
3	B	600	EST	O3-C3	2.43	1.42	1.37
3	A	600	EST	C11-C9	2.27	1.56	1.53
3	A	600	EST	C12-C11	2.09	1.57	1.53
3	A	600	EST	C15-C14	2.08	1.58	1.54
3	B	600	EST	C2-C3	2.06	1.42	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	600	EST	C14-C13-C17	-4.02	95.16	99.25
3	A	600	EST	C16-C17-C13	3.57	107.33	104.52
3	B	600	EST	C6-C7-C8	-2.94	105.70	110.61
3	A	600	EST	C11-C12-C13	-2.57	108.40	112.74
3	A	600	EST	C10-C9-C8	2.54	114.66	111.59
3	A	600	EST	C7-C8-C14	2.54	116.29	112.08
3	B	600	EST	C14-C13-C17	-2.38	96.83	99.25
3	A	600	EST	C2-C3-C4	-2.29	117.67	120.19
3	A	600	EST	C6-C7-C8	-2.29	106.78	110.61
3	A	600	EST	C15-C14-C13	2.28	106.52	103.84
3	A	600	EST	C5-C10-C9	-2.09	118.62	121.00
3	B	600	EST	C11-C9-C8	2.06	114.14	111.45
3	B	600	EST	C2-C3-C4	-2.03	117.96	120.19
3	B	600	EST	C7-C8-C14	2.03	115.45	112.08
3	B	600	EST	C9-C8-C14	-2.02	105.87	108.68

There are no chirality outliers.

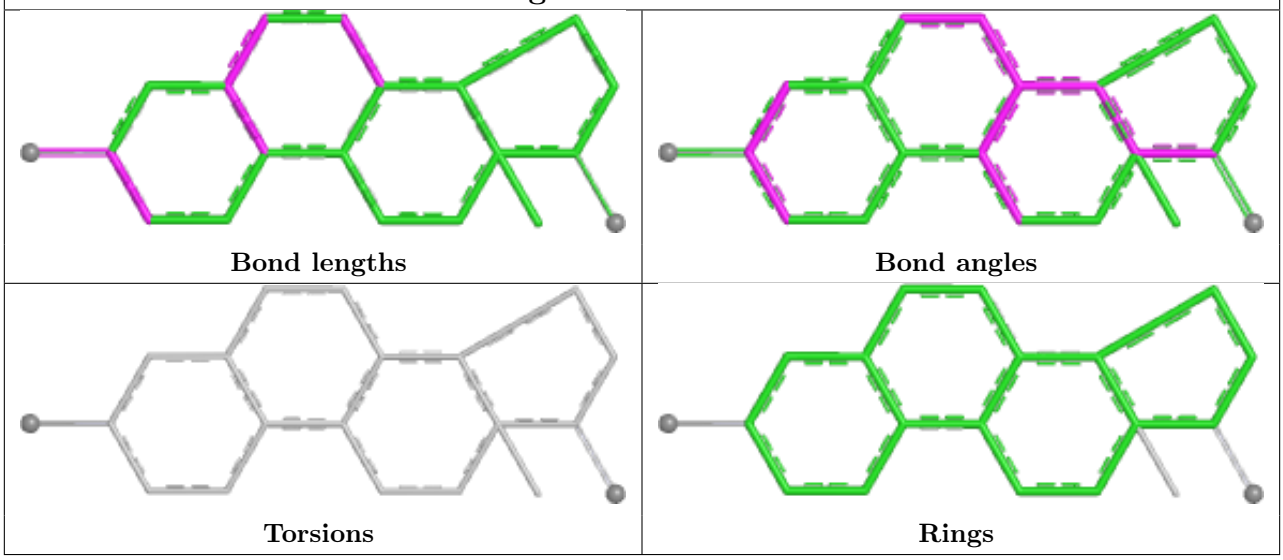
There are no torsion outliers.

There are no ring outliers.

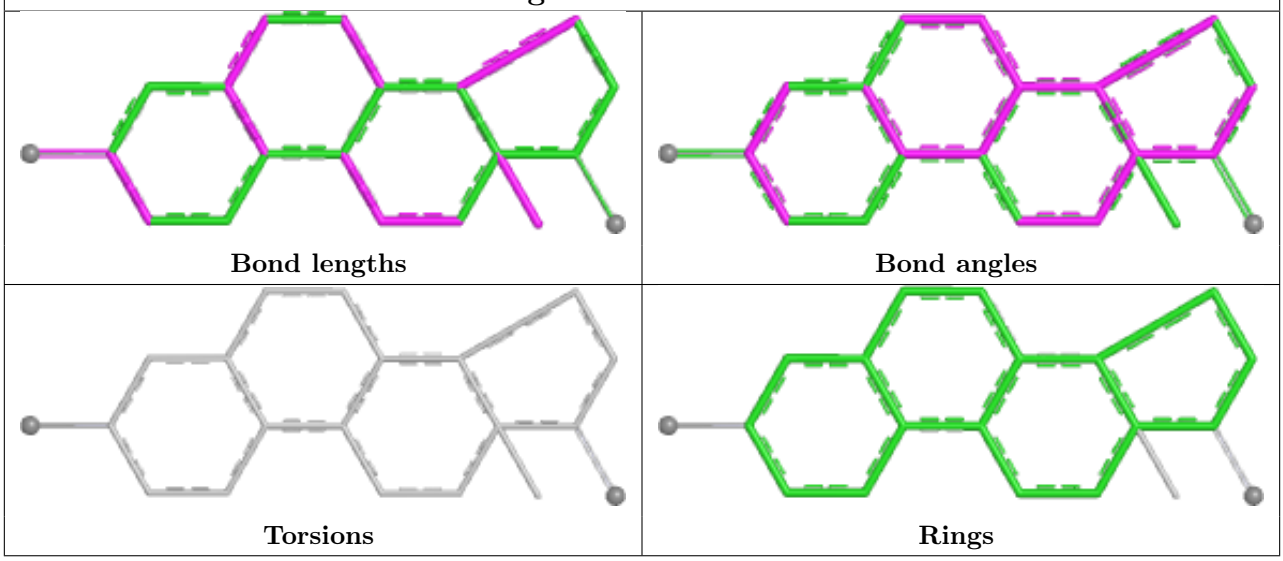
No monomer is involved in short contacts.

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 EST B 600



Ligand EST A 600



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	234/240 (97%)	-0.14	5 (2%) 63 68	12, 20, 33, 42	0
1	B	233/240 (97%)	-0.15	7 (3%) 50 55	12, 20, 33, 42	0
2	C	10/19 (52%)	0.90	3 (30%) 0 0	25, 29, 37, 43	0
2	D	10/19 (52%)	1.08	3 (30%) 0 0	26, 29, 39, 43	0
All	All	487/518 (94%)	-0.10	18 (3%) 41 46	12, 20, 34, 43	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	3	LYS	3.8
1	B	417	THR	3.8
2	D	3	LYS	3.7
1	A	497	ALA	3.4
1	A	412	PRO	3.3
1	B	497	ALA	3.0
1	B	410	MET	3.0
1	A	410	MET	2.9
2	D	4	ILE	2.8
2	C	4	ILE	2.8
1	A	417	THR	2.6
1	B	412	PRO	2.5
2	D	2	HIS	2.5
1	B	413	LEU	2.3
1	B	325[A]	PHE	2.2
1	A	481[A]	CYS	2.2
2	C	2	HIS	2.2
1	B	424	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PTR	A	488	16/17	0.90	0.14	27,31,44,44	0
1	PTR	B	488	16/17	0.92	0.14	27,31,44,44	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

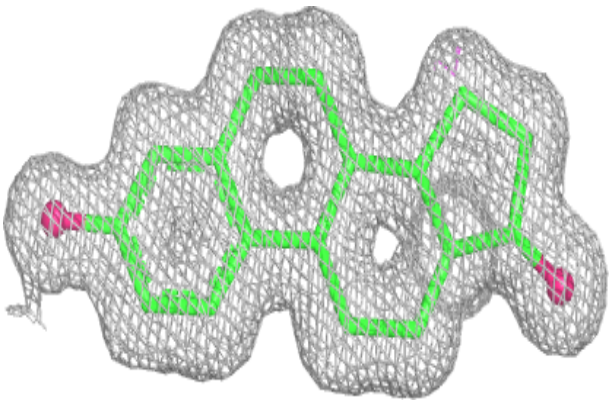
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

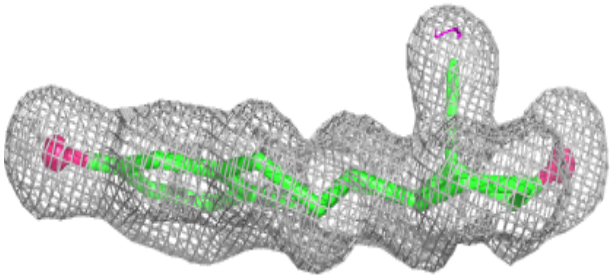
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EST	B	600	20/20	0.97	0.07	12,14,15,16	0
3	EST	A	600	20/20	0.98	0.07	13,14,16,16	0

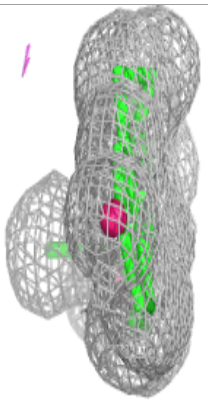
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EST 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)

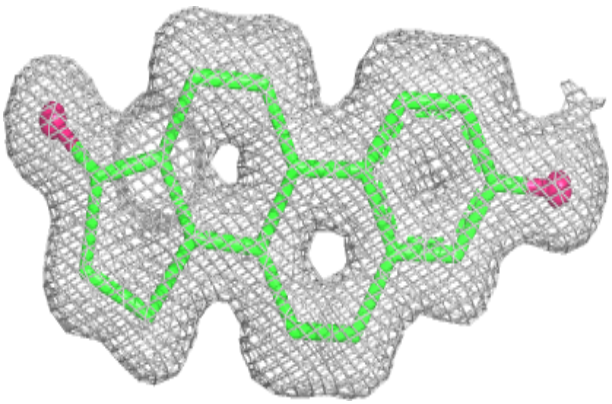


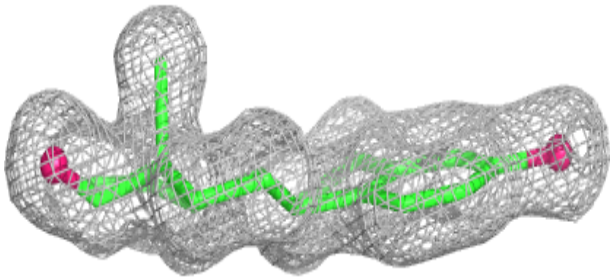


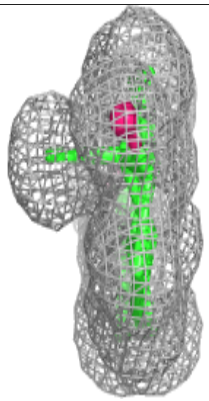


Electron density around EST A 600:

$2mF_o$-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.