



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:58 AM UTC

PDB ID : 3OLL / pdb_00003oll
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	:	4-5-2 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

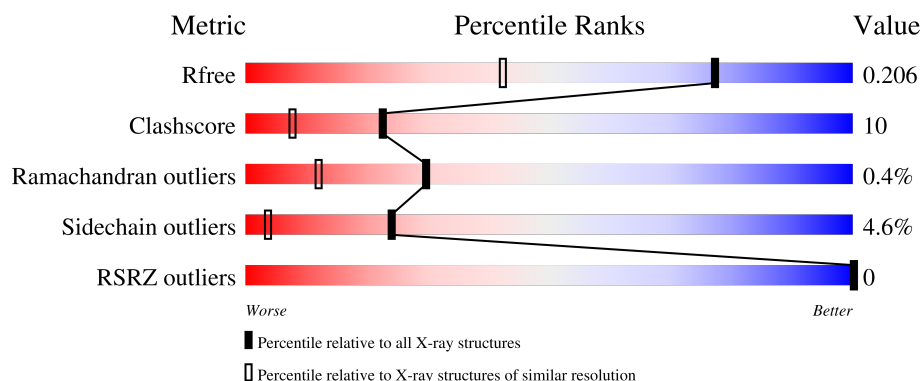
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 $\leq 5\%$. 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	240	
1	B	240	
2	C	19	
2	D	19	

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.

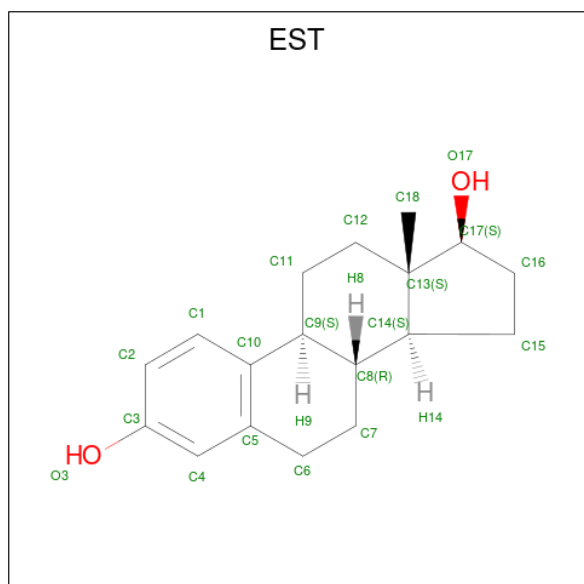
- Molecule 1 is a protein called Estrogen receptor beta.

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 (CCD ID: EST) (formula: C₁₈H₂₄O₂).



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

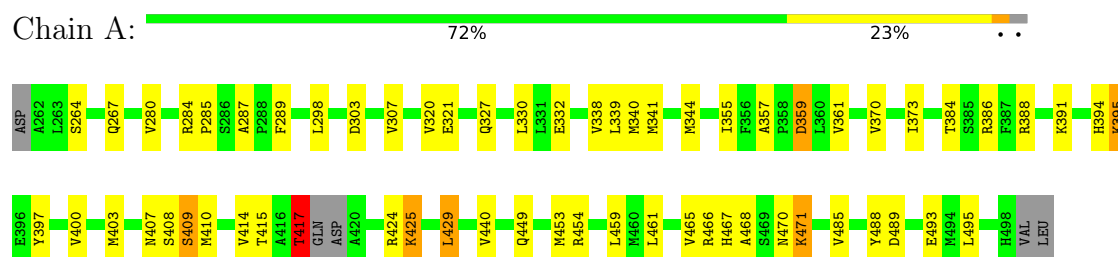
- Molecule 4 is water.

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

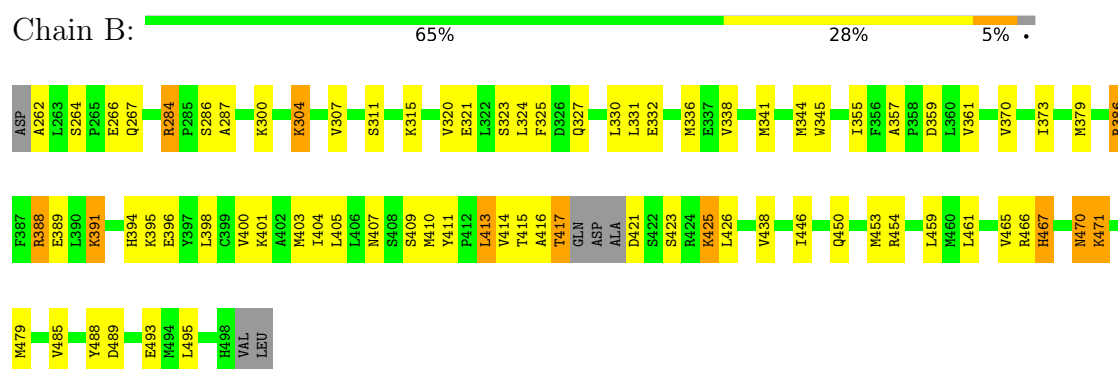
3 Residue-property plots

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.

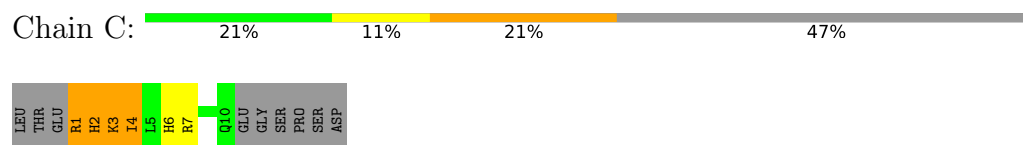
- Molecule 1: Estrogen receptor beta



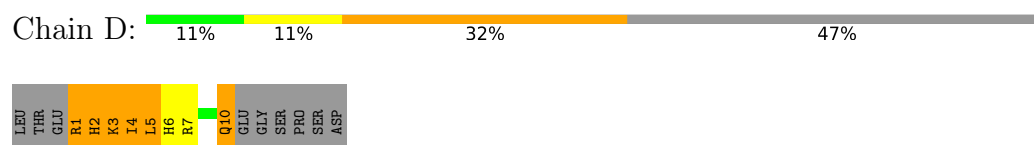
- Molecule 1: Estrogen receptor beta



- Molecule 2: Nuclear receptor coactivator 1



- Molecule 2: Nuclear receptor coactivator 1



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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: 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	2.17	40/1914 (2.1%)	1.24	11/2584 (0.4%)
1	B	2.20	50/1906 (2.6%)	1.39	20/2573 (0.8%)
2	C	2.47	5/93 (5.4%)	2.02	4/122 (3.3%)
2	D	2.67	7/93 (7.5%)	2.03	5/122 (4.1%)
All	All	2.21	102/4006 (2.5%)	1.36	40/5401 (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 (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	ARG	CD-NE	-13.14	1.27	1.46
2	D	4	ILE	CA-C	11.87	1.68	1.52
1	B	344	MET	SD-CE	-10.11	1.54	1.79
2	C	4	ILE	CA-C	9.96	1.66	1.53
1	A	344	MET	SD-CE	-9.70	1.55	1.79
1	B	304	LYS	CG-CD	-9.43	1.24	1.52
1	A	307	VAL	CA-CB	8.68	1.64	1.54
1	B	485	VAL	CA-CB	8.59	1.65	1.54
1	B	320	VAL	CA-CB	7.90	1.63	1.54
2	C	6	HIS	CA-C	-7.66	1.43	1.52
2	C	7	ARG	N-CA	-7.60	1.37	1.46
1	B	267	GLN	C-O	7.48	1.32	1.24
1	A	407	ASN	C-O	-7.39	1.12	1.23
1	A	287	ALA	CA-CB	-7.22	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	LYS	N-CA	7.11	1.55	1.46
1	A	341	MET	SD-CE	7.03	1.97	1.79
1	A	429	LEU	CG-CD1	-7.00	1.29	1.52
2	D	7	ARG	N-CA	-6.95	1.38	1.46
1	A	414	VAL	CA-CB	6.90	1.62	1.54
1	B	311	SER	N-CA	6.77	1.54	1.46
1	B	304	LYS	CB-CG	-6.70	1.32	1.52
1	B	370	VAL	CA-CB	6.66	1.62	1.54
1	A	417	THR	CA-CB	-6.63	1.36	1.54
1	B	284	ARG	NE-CZ	6.59	1.40	1.33
1	A	370	VAL	CA-CB	6.59	1.62	1.54
1	B	388	ARG	CD-NE	-6.52	1.37	1.46
1	B	341	MET	SD-CE	6.51	1.95	1.79
2	D	4	ILE	C-O	6.47	1.31	1.23
2	C	3	LYS	N-CA	6.38	1.54	1.46
1	B	338	VAL	CA-CB	6.38	1.62	1.54
1	A	357	ALA	N-CA	6.37	1.52	1.46
1	B	404	ILE	CA-CB	6.35	1.61	1.54
1	B	307	VAL	CA-CB	6.32	1.61	1.54
1	A	388	ARG	CD-NE	-6.30	1.37	1.46
1	B	409	SER	CA-C	-6.30	1.44	1.52
1	A	303	ASP	C-O	6.28	1.31	1.24
2	D	4	ILE	N-CA	6.25	1.54	1.46
1	A	495	LEU	C-O	-6.17	1.16	1.24
1	B	330	LEU	C-O	6.16	1.31	1.24
1	B	357	ALA	CA-CB	6.15	1.62	1.54
1	A	384	THR	N-CA	6.09	1.53	1.46
1	B	426	LEU	N-CA	6.02	1.53	1.46
1	A	485	VAL	CA-CB	5.98	1.61	1.54
1	B	401	LYS	CA-C	5.93	1.60	1.52
1	A	339	LEU	N-CA	5.91	1.53	1.46
1	A	407	ASN	C-N	-5.84	1.25	1.33
1	B	331	LEU	N-CA	5.82	1.53	1.46
1	B	286	SER	N-CA	5.82	1.53	1.46
1	A	327	GLN	C-O	5.82	1.30	1.24
1	A	465	VAL	CA-CB	5.77	1.61	1.54
1	A	320	VAL	CA-CB	5.77	1.62	1.54
1	A	340	MET	N-CA	5.74	1.53	1.46
1	B	414	VAL	N-CA	-5.74	1.39	1.46
1	A	453	MET	CA-C	5.74	1.60	1.52
1	A	267	GLN	C-O	5.73	1.30	1.24
1	A	397	TYR	C-O	5.71	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	438	VAL	CA-C	5.70	1.60	1.52
1	A	330	LEU	C-O	5.69	1.30	1.24
1	A	344	MET	N-CA	5.67	1.53	1.46
1	B	465	VAL	CA-CB	5.66	1.61	1.54
1	B	398	LEU	CA-C	5.64	1.60	1.52
1	B	407	ASN	C-N	-5.57	1.25	1.33
1	B	414	VAL	CA-CB	5.57	1.60	1.53
1	A	280	VAL	CA-C	5.56	1.59	1.52
2	C	4	ILE	N-CA	5.55	1.53	1.46
1	B	323	SER	C-O	5.54	1.30	1.23
1	A	407	ASN	CA-CB	5.52	1.60	1.52
1	B	266	GLU	C-O	5.51	1.30	1.24
2	D	6	HIS	CA-C	-5.50	1.45	1.52
1	B	336	MET	C-O	5.49	1.30	1.24
1	B	417	THR	C-O	5.47	1.34	1.23
1	B	453	MET	SD-CE	5.46	1.93	1.79
1	A	415	THR	N-CA	5.44	1.52	1.45
1	B	405	LEU	N-CA	5.41	1.52	1.46
1	B	396	GLU	CA-C	5.38	1.59	1.52
1	A	410	MET	C-O	5.37	1.29	1.23
1	A	338	VAL	CA-CB	5.36	1.61	1.54
1	B	495	LEU	C-O	-5.33	1.18	1.24
2	D	10	GLN	CB-CG	5.25	1.68	1.52
1	A	388	ARG	N-CA	5.25	1.52	1.46
1	A	408	SER	N-CA	5.25	1.51	1.45
1	A	320	VAL	CA-C	5.24	1.59	1.52
1	B	410	MET	CG-SD	-5.20	1.67	1.80
1	B	315	LYS	N-CA	5.19	1.52	1.46
1	B	479	MET	N-CA	5.19	1.52	1.46
1	A	298	LEU	C-O	5.19	1.30	1.24
1	B	467	HIS	CA-C	5.19	1.59	1.52
1	A	289	PHE	N-CA	5.16	1.52	1.46
1	B	287	ALA	CA-CB	-5.14	1.44	1.52
1	B	266	GLU	CA-C	5.13	1.59	1.52
1	B	345	TRP	CA-CB	5.12	1.61	1.53
1	B	400	VAL	CA-C	5.12	1.59	1.52
1	B	386	ARG	N-CA	5.11	1.52	1.46
1	A	285	PRO	CA-C	5.10	1.58	1.52
1	B	321	GLU	N-CA	5.07	1.52	1.46
1	A	468	ALA	C-O	5.06	1.30	1.24
1	B	417	THR	CA-C	-5.06	1.42	1.52
1	B	417	THR	CB-CG2	-5.06	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	327	GLN	C-O	5.01	1.29	1.24
1	B	470	ASN	CG-OD1	5.01	1.33	1.23
1	A	400	VAL	CA-C	5.00	1.59	1.52
1	A	440	VAL	CA-CB	5.00	1.60	1.54

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	ARG	NE-CZ-NH2	15.32	132.99	119.20
1	B	284	ARG	CD-NE-CZ	13.47	143.26	124.40
1	B	417	THR	CB-CA-C	-10.06	86.97	109.10
1	B	416	ALA	CA-C-N	9.99	139.67	121.70
1	B	416	ALA	C-N-CA	9.99	139.67	121.70
2	D	2	HIS	N-CA-C	-9.32	98.73	111.87
2	C	2	HIS	N-CA-C	-8.99	99.20	111.87
1	A	407	ASN	CA-C-N	-8.66	107.69	122.67
1	A	407	ASN	C-N-CA	-8.66	107.69	122.67
1	B	454	ARG	NE-CZ-NH2	8.32	126.69	119.20
1	B	284	ARG	NE-CZ-NH1	-8.27	113.23	121.50
1	B	389	GLU	CA-CB-CG	7.61	129.31	114.10
1	A	417	THR	CA-CB-OG1	-7.47	98.40	109.60
1	B	410	MET	N-CA-C	-7.20	101.80	110.44
1	A	284	ARG	NE-CZ-NH2	7.18	125.66	119.20
1	B	409	SER	CB-CA-C	-7.10	97.94	109.72
2	C	3	LYS	N-CA-C	6.98	125.66	110.80
1	A	454	ARG	NE-CZ-NH2	6.97	125.47	119.20
1	B	388	ARG	NE-CZ-NH2	-6.93	112.97	119.20
1	A	410	MET	N-CA-C	-6.82	100.31	110.06
2	D	3	LYS	N-CA-C	6.82	125.32	110.80
1	A	417	THR	CB-CA-C	-6.38	95.07	109.10
1	B	416	ALA	O-C-N	6.37	130.10	122.27
1	B	284	ARG	CG-CD-NE	-6.22	98.32	112.00
1	A	409	SER	CB-CA-C	-6.20	99.42	109.72
1	B	388	ARG	NE-CZ-NH1	6.18	127.68	121.50
1	B	411	TYR	CA-C-N	-6.14	113.62	119.76
1	B	411	TYR	C-N-CA	-6.14	113.62	119.76
2	D	4	ILE	CB-CA-C	-6.10	104.26	111.94
2	C	4	ILE	CB-CA-C	-5.97	103.23	111.65
2	D	4	ILE	CA-C-O	5.83	126.94	120.46
2	D	5	LEU	CD1-CG-CD2	5.77	123.50	110.80
1	B	388	ARG	CD-NE-CZ	5.63	132.28	124.40
2	C	7	ARG	N-CA-C	5.60	117.83	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	417	THR	N-CA-C	5.51	126.43	111.00
1	A	388	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	B	264	SER	N-CA-CB	-5.30	101.66	109.98
1	A	395	LYS	CB-CG-CD	5.28	123.44	111.30
1	A	359	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	423	SER	N-CA-C	5.12	116.86	111.28

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 ⓘ

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	30	0
1	B	1889	0	1948	44	1
2	C	92	0	107	18	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	10	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	86	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 (86) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:379:MET:HE1	1:B:467:HIS:ND1	1.88	0.88
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: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
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:B:403:MET:HE1	1:B:459:LEU:CD2	2.32	0.58
1:A:425:LYS:CG	4:A:560:HOH:O	2.51	0.58
1:A:417:THR:O	1:A:417:THR:CG2	2.29	0.57
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
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:403:MET:HE1	1:A:459:LEU:CD2	2.36	0.55
1:A:467:HIS:HD2	1:B:466:ARG:HD2	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:403:MET:HE1	1:B:459:LEU:HD22	1.92	0.52
1:B:493:GLU:CD	2:D:4:ILE:HB	2.34	0.51
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:B:379:MET:CE	1:B:467:HIS:ND1	2.69	0.49
1:B:493:GLU:CD	2:D:4:ILE:H	2.17	0.48
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
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
1:A:409:SER:HB2	4:A:598:HOH:O	2.16	0.45
1:A:403:MET:HE1	1:A:459:LEU:HD21	1.99	0.44
1:A:471:LYS:NZ	4:A:593:HOH:O	2.32	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:A:403:MET:HE1	1:A:459:LEU:HD22	2.00	0.43
1:A:493:GLU:CD	2:C:4:ILE:H	2.25	0.43
1:B:300:LYS:HE2	1:B:300:LYS:HB2	1.69	0.43
1:B:403:MET:HE1	1:B:459:LEU:HD21	2.01	0.42
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:471:LYS:CE	4:B:579:HOH:O	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	30	12
1	B	235/240 (98%)	228 (97%)	6 (3%)	1 (0%)	30	12
2	C	8/19 (42%)	7 (88%)	1 (12%)	0	100	100
2	D	8/19 (42%)	7 (88%)	1 (12%)	0	100	100
All	All	488/518 (94%)	473 (97%)	13 (3%)	2 (0%)	30	12

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%)	207 (96%)	9 (4%)	26	4
1	B	215/214 (100%)	207 (96%)	8 (4%)	30	6
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%)	431 (96%)	20 (4%)	24	4

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	SER
1	A	359	ASP
1	A	373	ILE
1	A	391	LYS
1	A	395	LYS
1	A	417	THR
1	A	425	LYS
1	A	449	GLN
1	A	471	LYS
1	B	304	LYS
1	B	359	ASP
1	B	373	ILE
1	B	391	LYS
1	B	395	LYS
1	B	413	LEU
1	B	425	LYS
1	B	471	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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	A	279	HIS
1	A	393	GLN

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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	B	267	GLN
1	B	394	HIS
1	B	407	ASN
1	B	428	HIS
1	B	470	ASN
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	B	488	1	15,16,17	1.69	4 (26%)	17,22,24	1.01	1 (5%)
1	PTR	A	488	1	15,16,17	1.82	2 (13%)	17,22,24	0.96	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	B	488	1	-	0/10/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	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(°)	Ideal(°)
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

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

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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

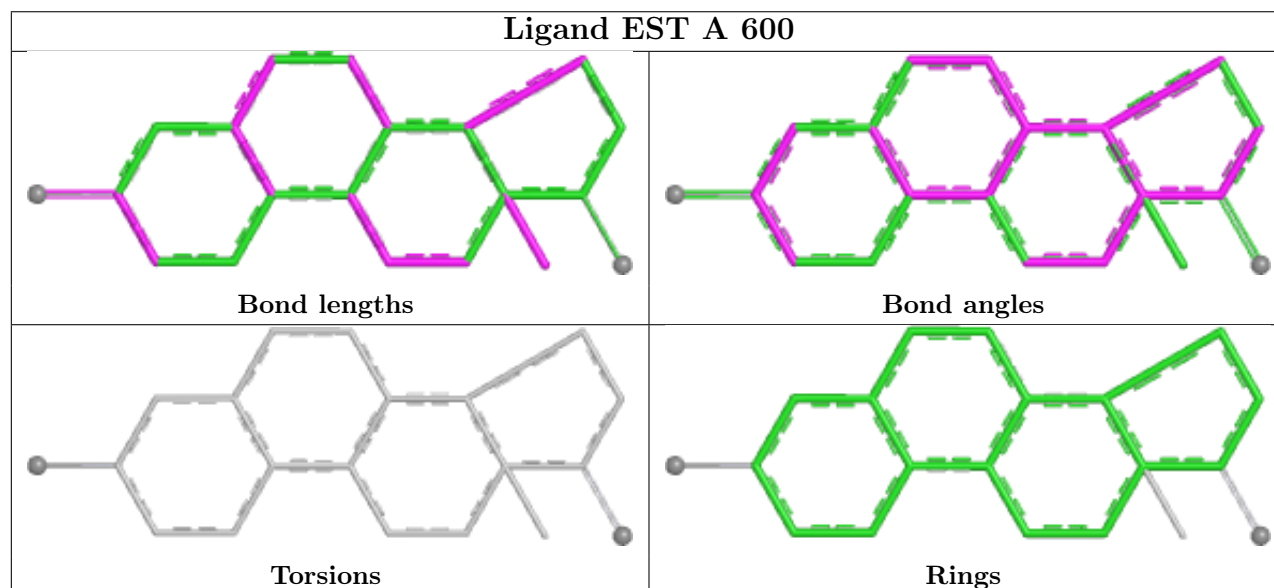
There are no chirality outliers.

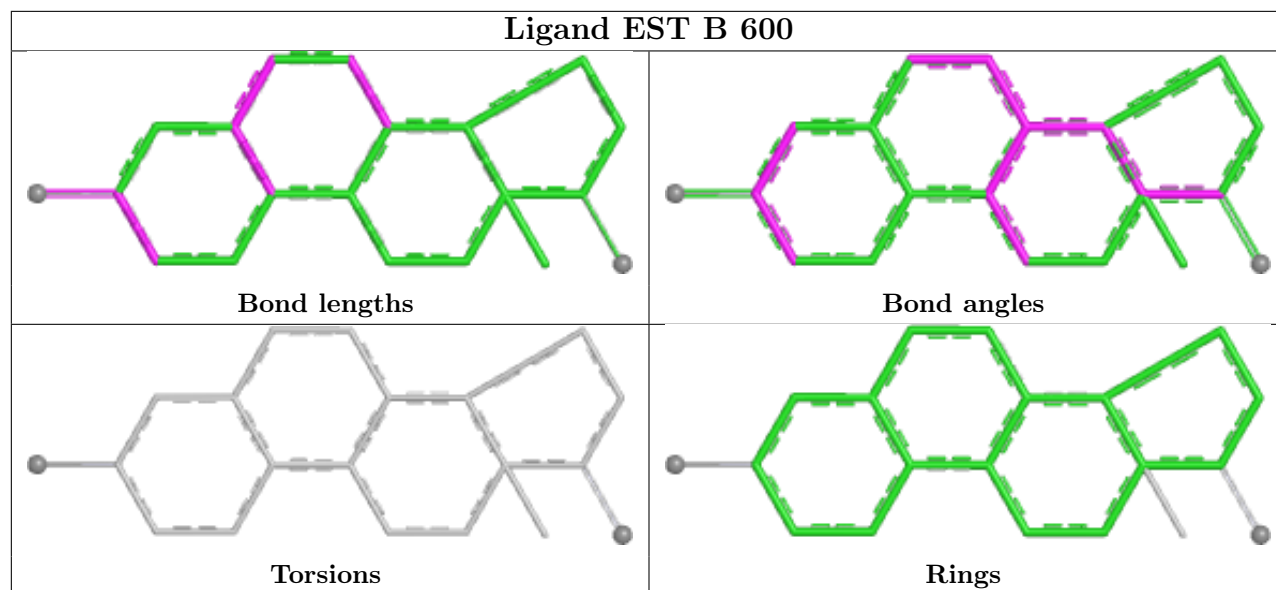
There are no torsion outliers.

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 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	234/240 (97%)	-1.16	0 100 100	8, 20, 33, 42	7 (2%)
1	B	233/240 (97%)	-1.16	0 100 100	8, 20, 33, 42	6 (2%)
2	C	10/19 (52%)	-0.53	0 100 100	25, 29, 37, 43	0
2	D	10/19 (52%)	-0.47	0 100 100	26, 29, 39, 43	0
All	All	487/518 (94%)	-1.13	0 100 100	8, 20, 34, 43	13 (2%)

There are no RSRZ outliers to report.

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, 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
1	PTR	A	488	16/17	0.98	0.05	27,31,44,44	0
1	PTR	B	488	16/17	0.98	0.06	27,31,44,44	0

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

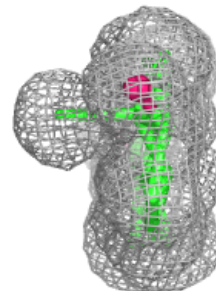
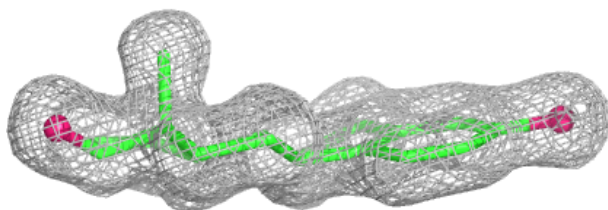
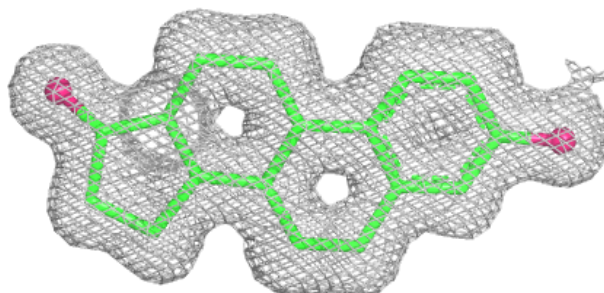
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EST	A	600	20/20	0.99	0.02	13,14,16,16	0
3	EST	B	600	20/20	0.99	0.03	12,14,15,16	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.

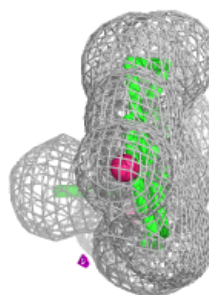
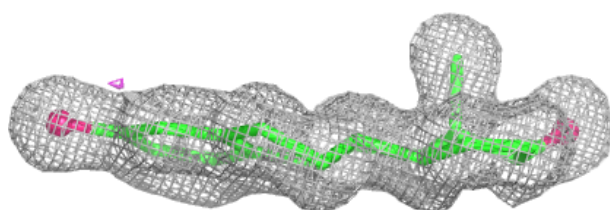
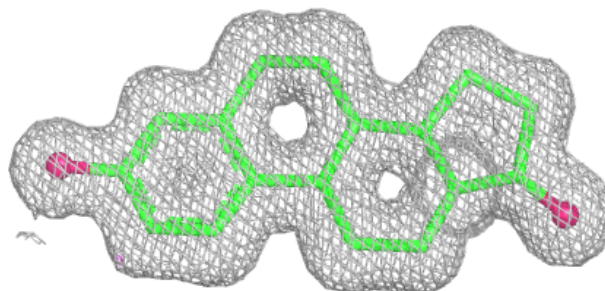
Electron density around EST A 600:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.