



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2022 – 01:23 pm BST

PDB ID : 7NEL
Title : ER-PRS*(+) (Y537S) in complex with estradiol and SRC-2 coactivator peptide
Authors : Kriegel, M.; Muller, Y.A.
Deposited on : 2021-02-04
Resolution : 1.45 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 : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

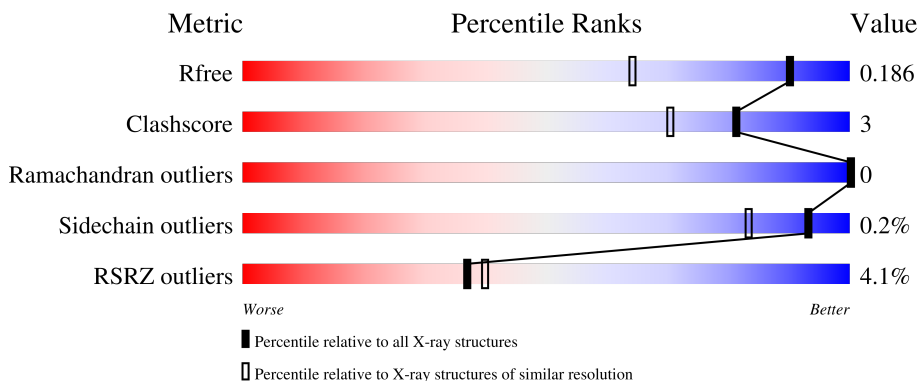
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	247	 3% 92% 6%
1	B	247	 4% 92% 7%
2	C	15	 13% 60% 20% 20%
2	D	15	 13% 73% 7% 20%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9320 atoms, of which 4535 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	242	4022	1278	2040	329	359	16	0	8	0
1	B	245	4119	1310	2091	337	364	17	0	11	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	SER	-	expression tag	UNP P03372
A	303	MET	-	expression tag	UNP P03372
A	315	ILE	MET	engineered mutation	UNP P03372
A	316	ILE	VAL	engineered mutation	UNP P03372
A	321	GLU	ASP	engineered mutation	UNP P03372
A	334	SER	THR	engineered mutation	UNP P03372
A	341	TYR	SER	engineered mutation	UNP P03372
A	363	LYS	ARG	engineered mutation	UNP P03372
A	371	SER	THR	engineered mutation	UNP P03372
A	381	SER	CYS	engineered mutation	UNP P03372
A	397	ASP	GLU	engineered mutation	UNP P03372
A	407	ASP	ASN	engineered mutation	UNP P03372
A	413	GLU	ASN	engineered mutation	UNP P03372
A	417	SER	CYS	engineered mutation	UNP P03372
A	433	GLU	SER	engineered mutation	UNP P03372
A	437	GLU	MET	engineered mutation	UNP P03372
A	439	LYS	ASN	engineered mutation	UNP P03372
A	442	ARG	GLY	engineered mutation	UNP P03372
A	450	ALA	SER	engineered mutation	UNP P03372
A	471	ASN	GLU	engineered mutation	UNP P03372
A	473	GLU	ASP	engineered mutation	UNP P03372
A	474	LYS	HIS	engineered mutation	UNP P03372
A	478	MET	VAL	engineered mutation	UNP P03372
A	485	ALA	THR	engineered mutation	UNP P03372
A	488	TRP	HIS	engineered mutation	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
A	489	TYR	LEU	engineered mutation	UNP P03372
A	493	SER	ALA	engineered mutation	UNP P03372
A	496	SER	THR	engineered mutation	UNP P03372
A	530	SER	CYS	engineered mutation	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372
B	302	SER	-	expression tag	UNP P03372
B	303	MET	-	expression tag	UNP P03372
B	315	ILE	MET	engineered mutation	UNP P03372
B	316	ILE	VAL	engineered mutation	UNP P03372
B	321	GLU	ASP	engineered mutation	UNP P03372
B	334	SER	THR	engineered mutation	UNP P03372
B	341	TYR	SER	engineered mutation	UNP P03372
B	363	LYS	ARG	engineered mutation	UNP P03372
B	371	SER	THR	engineered mutation	UNP P03372
B	381	SER	CYS	engineered mutation	UNP P03372
B	397	ASP	GLU	engineered mutation	UNP P03372
B	407	ASP	ASN	engineered mutation	UNP P03372
B	413	GLU	ASN	engineered mutation	UNP P03372
B	417	SER	CYS	engineered mutation	UNP P03372
B	433	GLU	SER	engineered mutation	UNP P03372
B	437	GLU	MET	engineered mutation	UNP P03372
B	439	LYS	ASN	engineered mutation	UNP P03372
B	442	ARG	GLY	engineered mutation	UNP P03372
B	450	ALA	SER	engineered mutation	UNP P03372
B	471	ASN	GLU	engineered mutation	UNP P03372
B	473	GLU	ASP	engineered mutation	UNP P03372
B	474	LYS	HIS	engineered mutation	UNP P03372
B	478	MET	VAL	engineered mutation	UNP P03372
B	485	ALA	THR	engineered mutation	UNP P03372
B	488	TRP	HIS	engineered mutation	UNP P03372
B	489	TYR	LEU	engineered mutation	UNP P03372
B	493	SER	ALA	engineered mutation	UNP P03372
B	496	SER	THR	engineered mutation	UNP P03372
B	530	SER	CYS	engineered mutation	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

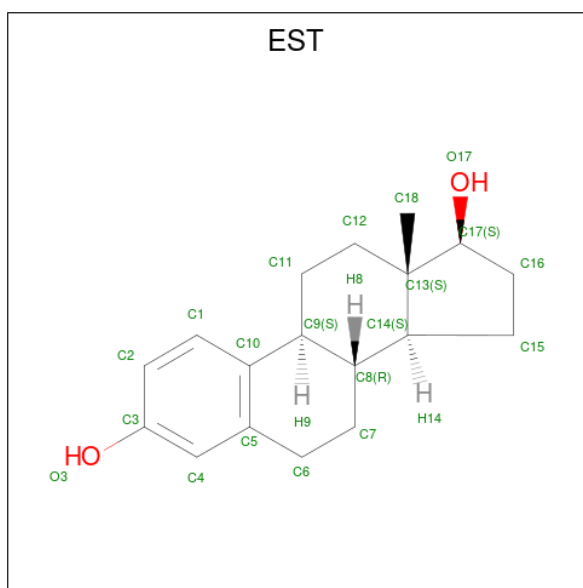
- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	H	N	O	0	1	0
			225	68	116	24	17			
2	D	12	Total	C	H	N	O	0	1	0
			229	70	120	24	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	685	ACE	-	acetylation	UNP Q15596
D	685	ACE	-	acetylation	UNP Q15596

- Molecule 3 is ESTRADIOL (three-letter code: EST) (formula: $C_{18}H_{24}O_2$) (labeled as "Ligand of Interest" by depositor).



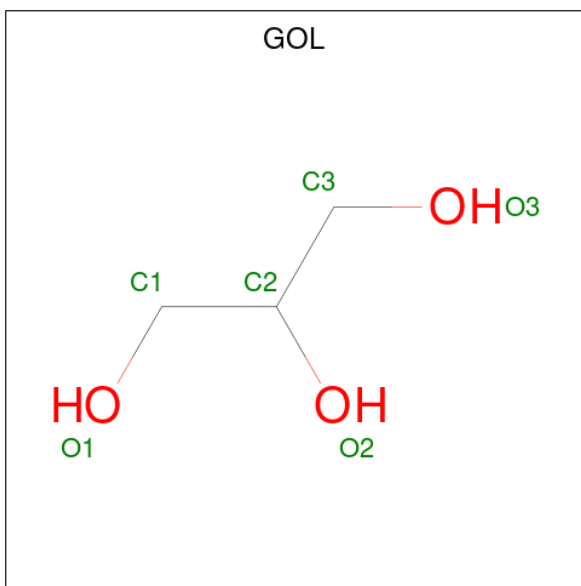
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
3	A	1	Total	C	H	O	0	0
			44	18	24	2		
3	B	1	Total	C	H	O	0	0
			44	18	24	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			13	3	7	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			13	3	7	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			12	3	6	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

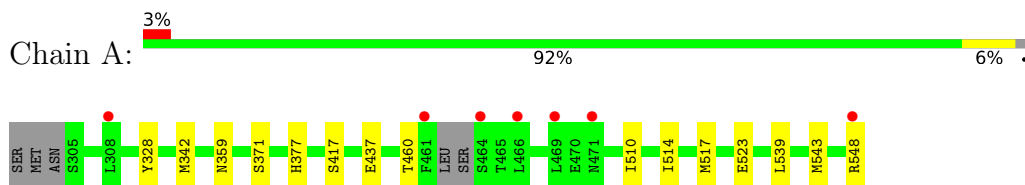
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	209	Total 209	O 209	0	0
8	B	210	Total 210	O 210	0	0
8	C	5	Total 5	O 5	0	0
8	D	5	Total 5	O 5	0	0

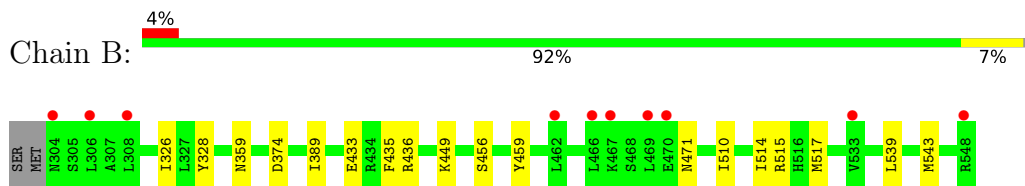
3 Residue-property plots [i](#)

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.

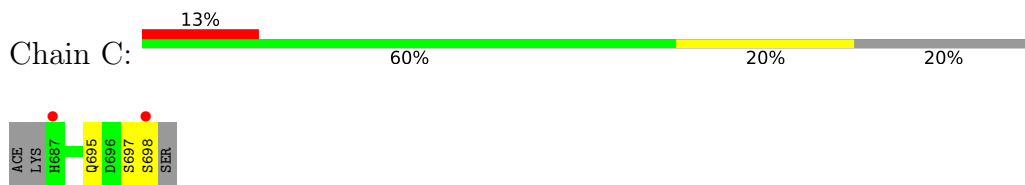
- Molecule 1: Estrogen receptor



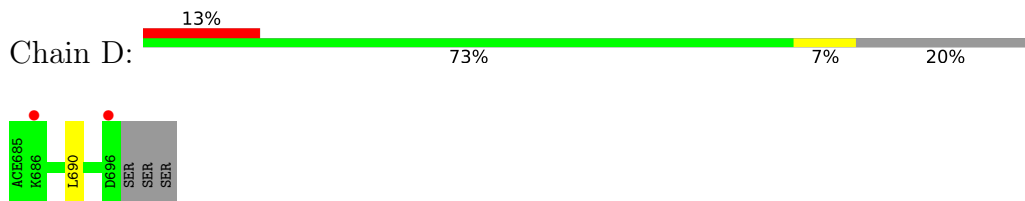
- Molecule 1: Estrogen receptor



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.80Å 82.77Å 58.69Å 90.00° 108.82° 90.00°	Depositor
Resolution (Å)	26.41 – 1.45 46.13 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.4 (26.41-1.45) 99.5 (46.13-1.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.149 , 0.186 0.149 , 0.186	Depositor DCC
R_{free} test set	1946 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9320	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, EDO, GOL, NA, CL, EST

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	0.34	0/2043	0.53	0/2754
1	B	0.32	0/2104	0.50	0/2838
2	C	0.29	0/113	0.56	0/149
2	D	0.23	0/111	0.43	0/146
All	All	0.33	0/4371	0.52	0/5887

There are no bond length outliers.

There are no bond angle outliers.

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	1982	2040	2054	11	3
1	B	2028	2091	2111	11	3
2	C	109	116	118	2	0
2	D	109	120	125	2	0
3	A	20	24	24	0	0
3	B	20	24	24	0	0
4	A	36	54	54	1	0
4	B	20	30	30	1	0
5	A	30	36	40	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	B	1	0	0	0	0
8	A	209	0	0	3	0
8	B	210	0	0	0	0
8	C	5	0	0	1	0
8	D	5	0	0	0	0
All	All	4785	4535	4580	23	3

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 3.

All (23) 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:523[A]:GLU:OE1	8:A:701:HOH:O	1.87	0.90
1:B:433:GLU:OE1	1:B:436:ARG:NH1	2.18	0.77
2:C:695:GLN:OE1	8:C:701:HOH:O	2.05	0.73
1:A:523[A]:GLU:OE2	8:A:702:HOH:O	2.15	0.64
1:A:359[A]:ASN:OD1	4:A:605:EDO:O2	2.12	0.64
1:A:377:HIS:CE1	1:A:460:THR:HG21	2.33	0.64
1:B:374:ASP:OD2	1:B:471:ASN:ND2	2.31	0.61
1:A:514[A]:ILE:HD13	1:A:517:MET:CE	2.34	0.57
1:B:326:ILE:HD11	4:B:608:EDO:H11	1.88	0.55
1:A:548:ARG:NH1	8:A:705:HOH:O	2.41	0.54
1:A:377:HIS:NE2	1:A:460:THR:HG21	2.22	0.53
1:B:456:SER:HA	1:B:515:ARG:NH2	2.25	0.51
1:A:510:ILE:HG12	1:B:459:TYR:OH	2.12	0.49
1:A:437:GLU:CD	5:A:612:GOL:HO3	2.13	0.48
2:C:697:SER:O	2:C:698:SER:CB	2.61	0.48
1:A:539:LEU:O	1:A:543:MET:HG2	2.14	0.48
1:B:514[A]:ILE:HD13	1:B:517:MET:CE	2.44	0.47
1:B:543[B]:MET:HE2	2:D:690:LEU:HD13	2.00	0.44
1:A:342[A]:MET:SD	1:A:417[A]:SER:OG	2.77	0.43
1:B:435:PHE:HE1	1:B:510:ILE:HG21	1.84	0.43
1:B:543[B]:MET:CE	2:D:690:LEU:HD13	2.49	0.43
1:B:539:LEU:O	1:B:543[A]:MET:HG2	2.22	0.40
1:B:389:ILE:HG21	1:B:449:LYS:HG2	2.03	0.40

All (3) 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:A:328:TYR:OH	1:B:359[A]:ASN:HD21[1_554]	1.33	0.27
1:A:359[A]:ASN:HD21	1:B:328:TYR:OH[1_554]	1.51	0.09
1:A:328:TYR:OH	1:B:359[A]:ASN:ND2[1_554]	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	246/247 (100%)	245 (100%)	1 (0%)	0	100	100
1	B	255/247 (103%)	255 (100%)	0	0	100	100
2	C	11/15 (73%)	11 (100%)	0	0	100	100
2	D	11/15 (73%)	11 (100%)	0	0	100	100
All	All	523/524 (100%)	522 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/223 (101%)	225 (100%)	1 (0%)	91	80
1	B	233/223 (104%)	233 (100%)	0	100	100
2	C	13/14 (93%)	13 (100%)	0	100	100
2	D	12/14 (86%)	12 (100%)	0	100	100
All	All	484/474 (102%)	483 (100%)	1 (0%)	93	83

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

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	$\# Z > 2$
4	EDO	A	609	-	3,3,3	0.43	0	2,2,2	0.11	0
5	GOL	A	612	-	5,5,5	0.95	0	5,5,5	0.94	0
5	GOL	A	611	-	5,5,5	1.06	0	5,5,5	0.79	0
5	GOL	A	614	-	5,5,5	0.84	0	5,5,5	0.90	0
4	EDO	B	608	-	3,3,3	0.47	0	2,2,2	0.20	0
4	EDO	A	610	-	3,3,3	0.51	0	2,2,2	0.17	0
4	EDO	A	604	-	3,3,3	0.41	0	2,2,2	0.33	0
4	EDO	A	603	-	3,3,3	0.47	0	2,2,2	0.28	0
4	EDO	A	607	-	3,3,3	0.44	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	604	-	3,3,3	0.41	0	2,2,2	0.20	0
4	EDO	A	602	-	3,3,3	0.43	0	2,2,2	0.09	0
4	EDO	A	606	-	3,3,3	0.47	0	2,2,2	0.38	0
5	GOL	A	615	-	5,5,5	1.01	0	5,5,5	0.90	0
4	EDO	B	606	-	3,3,3	0.50	0	2,2,2	0.09	0
3	EST	B	601	-	23,23,23	1.01	2 (8%)	36,36,36	1.07	2 (5%)
4	EDO	A	608	-	3,3,3	0.46	0	2,2,2	0.27	0
5	GOL	A	613	-	5,5,5	0.98	0	5,5,5	0.84	0
4	EDO	B	607	-	3,3,3	0.44	0	2,2,2	0.32	0
4	EDO	A	605	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	B	605	-	3,3,3	0.46	0	2,2,2	0.27	0
3	EST	A	601	-	23,23,23	1.19	2 (8%)	36,36,36	0.97	2 (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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	609	-	-	1/1/1/1	-
5	GOL	A	612	-	-	2/4/4/4	-
5	GOL	A	611	-	-	4/4/4/4	-
5	GOL	A	614	-	-	2/4/4/4	-
4	EDO	B	608	-	-	0/1/1/1	-
4	EDO	A	610	-	-	1/1/1/1	-
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	A	603	-	-	0/1/1/1	-
4	EDO	A	607	-	-	0/1/1/1	-
4	EDO	B	604	-	-	0/1/1/1	-
4	EDO	A	602	-	-	0/1/1/1	-
4	EDO	A	606	-	-	0/1/1/1	-
5	GOL	A	615	-	-	2/4/4/4	-
4	EDO	B	606	-	-	0/1/1/1	-
3	EST	B	601	-	-	-	0/4/4/4
4	EDO	A	608	-	-	0/1/1/1	-
5	GOL	A	613	-	-	0/4/4/4	-
4	EDO	B	607	-	-	1/1/1/1	-
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	B	605	-	-	1/1/1/1	-
3	EST	A	601	-	-	-	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	EST	O17-C17	-3.32	1.38	1.43
3	B	601	EST	O17-C17	-2.63	1.39	1.43
3	B	601	EST	C13-C17	2.32	1.57	1.54
3	A	601	EST	C13-C17	2.28	1.57	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	EST	C16-C17-C13	-2.95	102.19	104.53
3	A	601	EST	C16-C17-C13	-2.83	102.28	104.53
3	B	601	EST	C13-C14-C8	-2.33	110.92	114.38
3	A	601	EST	C11-C9-C8	-2.05	108.63	111.39

There are no chirality outliers.

All (14) torsion outliers are listed below:

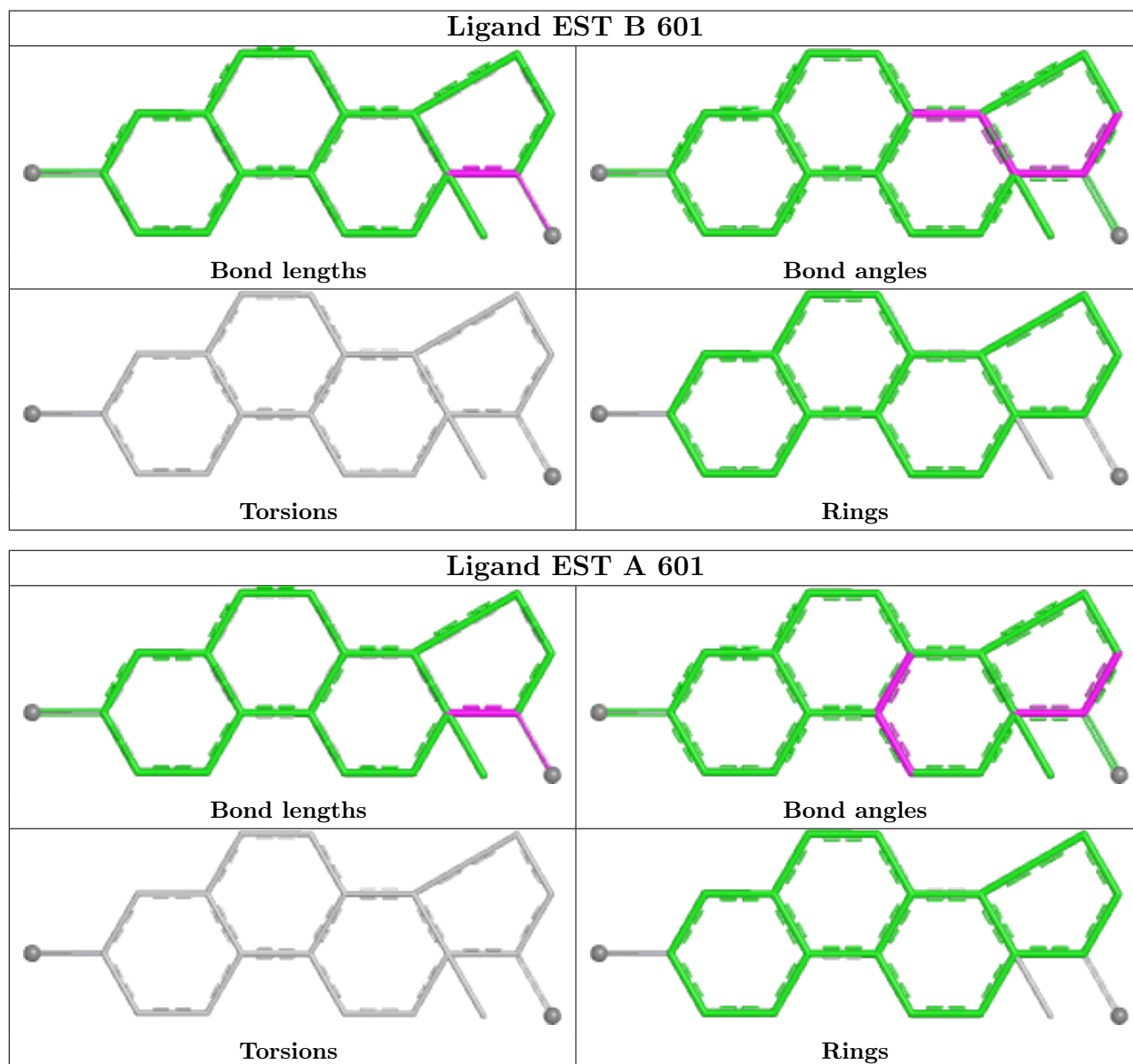
Mol	Chain	Res	Type	Atoms
5	A	614	GOL	O1-C1-C2-C3
5	A	614	GOL	O1-C1-C2-O2
5	A	611	GOL	O1-C1-C2-C3
5	A	611	GOL	C1-C2-C3-O3
5	A	612	GOL	C1-C2-C3-O3
5	A	615	GOL	O1-C1-C2-C3
5	A	611	GOL	O1-C1-C2-O2
5	A	611	GOL	O2-C2-C3-O3
5	A	612	GOL	O2-C2-C3-O3
4	A	610	EDO	O1-C1-C2-O2
4	A	609	EDO	O1-C1-C2-O2
5	A	615	GOL	O1-C1-C2-O2
4	B	607	EDO	O1-C1-C2-O2
4	B	605	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	612	GOL	1	0
4	B	608	EDO	1	0
4	A	605	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	242/247 (97%)	-0.26	7 (2%) 51 53	17, 25, 61, 95	0
1	B	245/247 (99%)	-0.11	10 (4%) 37 40	19, 29, 61, 85	0
2	C	12/15 (80%)	0.57	2 (16%) 1 2	23, 35, 86, 95	0
2	D	11/15 (73%)	0.54	2 (18%) 1 1	33, 40, 76, 80	0
All	All	510/524 (97%)	-0.15	21 (4%) 37 40	17, 28, 65, 95	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	LEU	6.9
1	B	304	ASN	4.6
1	B	467	LYS	4.3
1	B	548	ARG	3.4
1	A	461	PHE	3.4
1	B	533	VAL	3.3
1	A	548	ARG	3.0
1	A	469	LEU	2.8
1	B	470	GLU	2.8
1	B	462	LEU	2.7
1	B	469	LEU	2.7
2	D	696	ASP	2.7
1	B	308	LEU	2.5
1	A	464	SER	2.3
1	A	471	ASN	2.3
2	C	698	SER	2.2
1	A	308	LEU	2.2
2	C	687	HIS	2.1
1	A	466	LEU	2.1
1	B	306	LEU	2.1
2	D	686	LYS	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 monosaccharides in this entry.

6.4 Ligands [i](#)

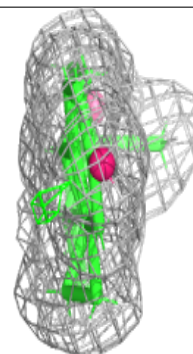
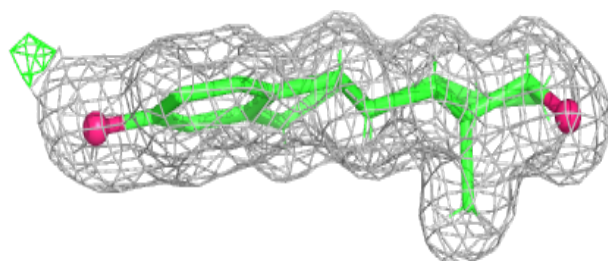
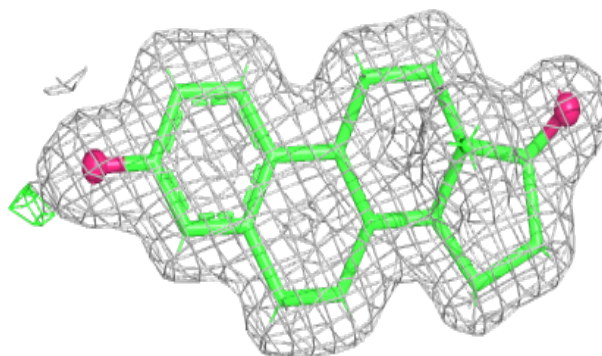
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	614	6/6	0.69	0.21	67,81,83,83	0
5	GOL	A	613	6/6	0.72	0.28	63,65,77,77	0
5	GOL	A	612	6/6	0.72	0.21	74,89,91,91	0
4	EDO	A	608	4/4	0.75	0.16	71,86,86,86	0
4	EDO	A	606	4/4	0.75	0.10	58,70,70,70	0
4	EDO	A	603	4/4	0.79	0.27	60,72,73,74	0
4	EDO	A	609	4/4	0.83	0.21	54,65,70,71	0
4	EDO	B	608	4/4	0.84	0.35	63,76,77,77	0
4	EDO	A	607	4/4	0.84	0.18	63,76,78,78	0
4	EDO	A	602	4/4	0.85	0.24	39,47,49,51	0
5	GOL	A	615	6/6	0.85	0.45	61,64,77,77	0
4	EDO	B	607	4/4	0.86	0.24	51,62,63,64	0
5	GOL	A	611	6/6	0.86	0.16	48,52,62,62	0
4	EDO	B	605	4/4	0.88	0.14	35,42,48,48	0
4	EDO	A	605	4/4	0.89	0.12	56,68,68,69	0
4	EDO	A	610	4/4	0.91	0.17	36,44,48,49	0
4	EDO	B	604	4/4	0.92	0.24	45,54,58,59	0
4	EDO	B	606	4/4	0.95	0.09	33,40,44,44	0
3	EST	B	601	20/20	0.97	0.08	22,27,31,32	0
4	EDO	A	604	4/4	0.97	0.06	33,40,43,44	0
3	EST	A	601	20/20	0.98	0.08	16,22,24,25	0
6	NA	B	602	1/1	0.99	0.06	27,27,27,27	0
7	CL	B	603	1/1	1.00	0.06	25,25,25,25	0

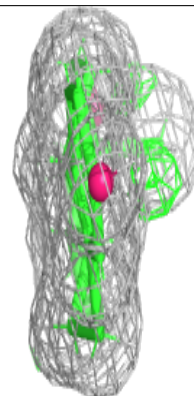
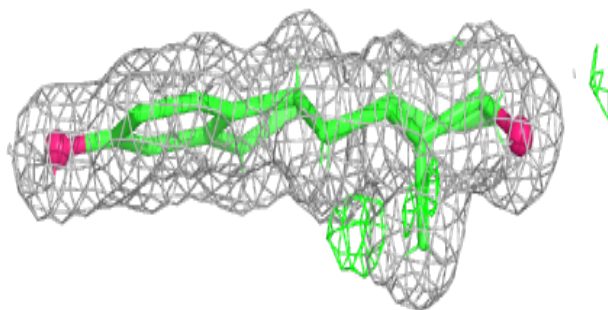
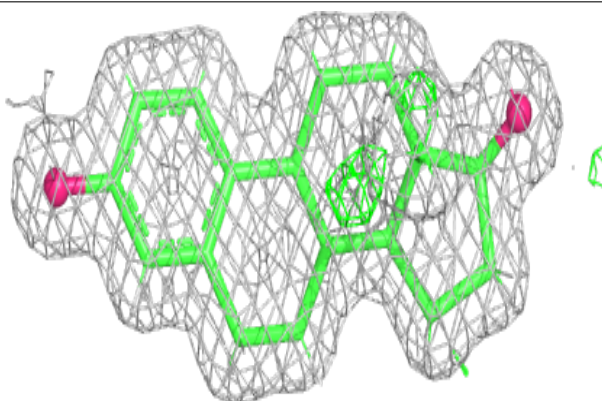
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EST B 601:

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

**Electron density around EST A 601:**

$2mF_o-DF_c$ (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.