



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:07 am BST

PDB ID : 4FN9
Title : X-ray Crystal structure of the Ancestral 3-keto steroid receptor - Progesterone complex
Authors : Colucci, J.K.; Ortlund, E.A.; Thornton, J.W.
Deposited on : 2012-06-19
Resolution : 3.00 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

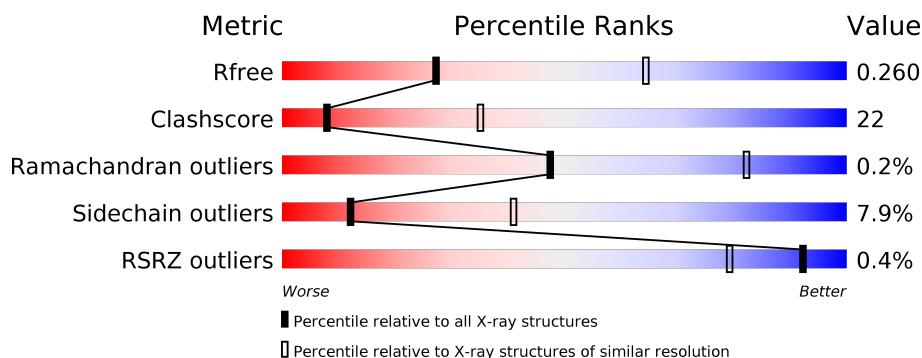
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 $\leq 5\%$. 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	254	 61% 32% 6% .
1	B	254	 56% 39% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	STR	A	301	-	-	X	-
2	STR	B	301	-	-	X	-

2 Entry composition [i](#)

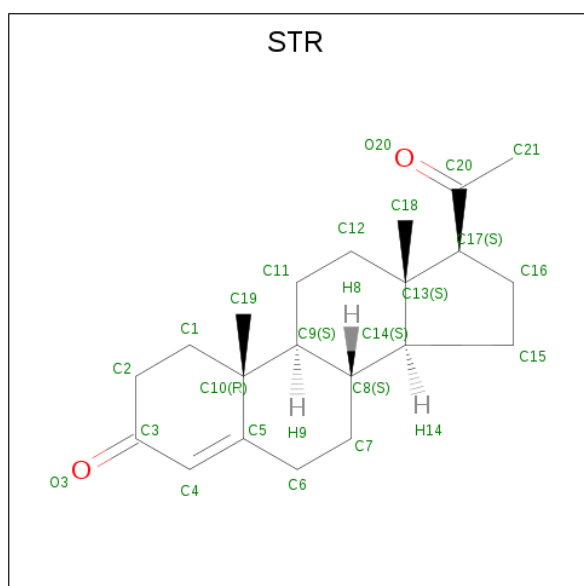
There are 7 unique types of molecules in this entry. The entry contains 4175 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Steroid receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			2018	1299	335	367	17			
1	B	249	Total	C	N	O	S	0	0	0
			2009	1293	333	366	17			

- Molecule 2 is PROGESTERONE (three-letter code: STR) (formula: $C_{21}H_{30}O_2$).



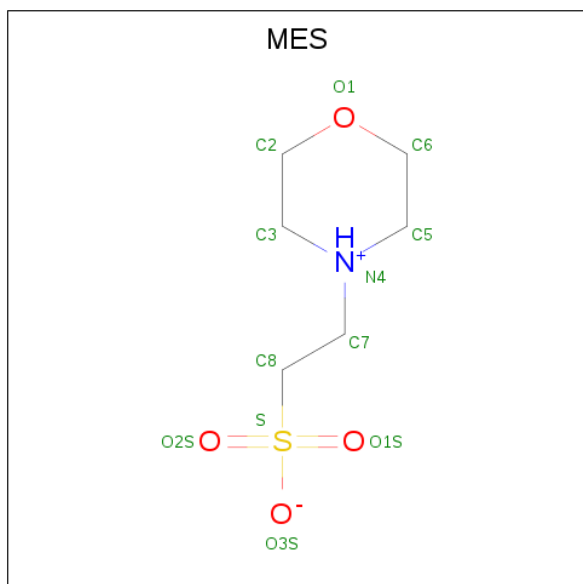
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	21	2		
2	B	1	Total	C	O	0	0
			23	21	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



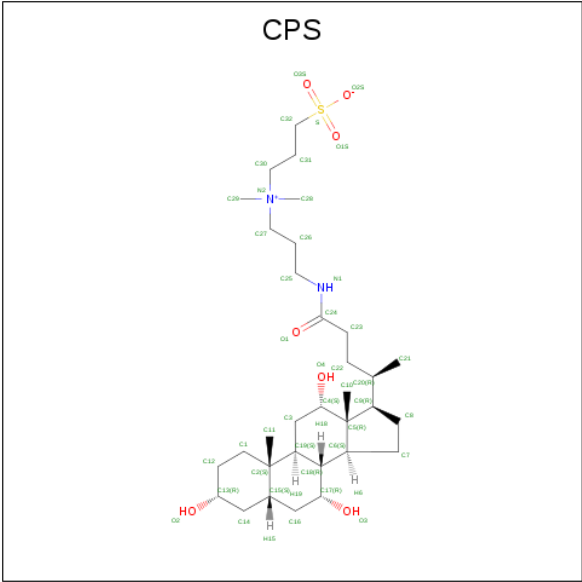
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	12	6	1	4	1	0	0

- Molecule 5 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: C₃₂H₅₈N₂O₇S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	23	20	3	0	0
5	B	1	25	22	3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

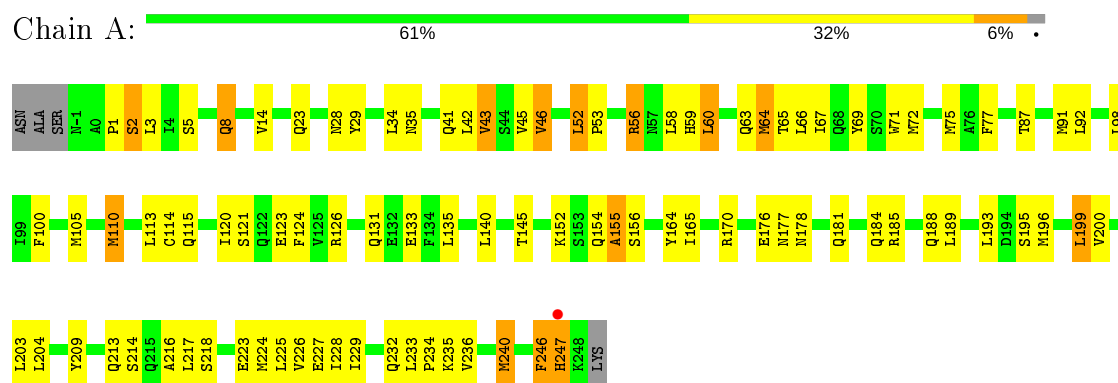
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total	O	0	0
			8	8		
7	B	5	Total	O	0	0
			5	5		

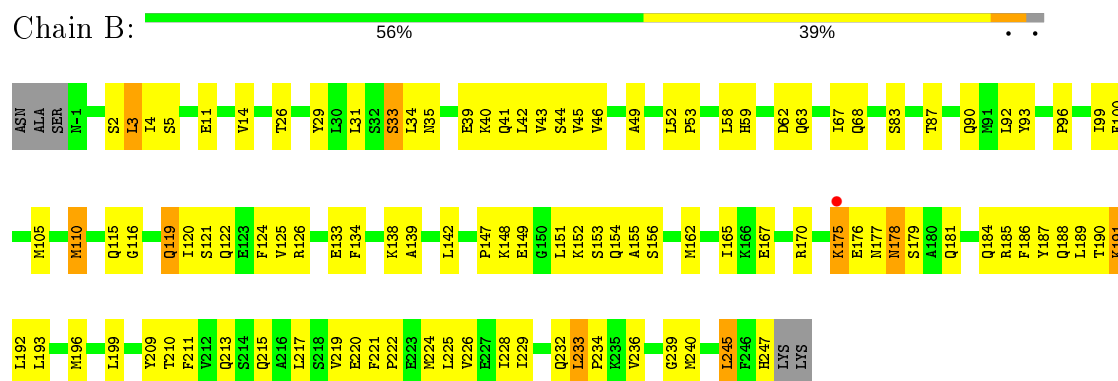
3 Residue-property plots [i](#)

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: Steroid receptor 2



• Molecule 1: Steroid receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.47Å 112.11Å 132.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 3.00 49.60 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.60-3.00) 100.0 (49.60-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.63 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1_743, REFMAC 5.5.0110	Depositor
R, R_{free}	0.203 , 0.260 0.202 , 0.260	Depositor DCC
R_{free} test set	857 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4175	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4206e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: STR, GOL, CPS, SO4, MES

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	0.49	0/2061	0.62	0/2784
1	B	0.47	0/2052	0.61	0/2773
All	All	0.48	0/4113	0.62	0/5557

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	PHE	Peptide

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	2018	0	2028	78	0
1	B	2009	0	2015	96	0
2	A	23	0	30	11	0
2	B	23	0	30	9	0
3	A	12	0	16	0	0
4	A	12	0	12	1	0
4	B	12	0	12	2	0
5	A	23	0	31	6	0
5	B	25	0	35	1	0
6	A	5	0	0	0	0
7	A	8	0	0	1	0
7	B	5	0	0	1	0
All	All	4175	0	4209	180	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (180) 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:209:TYR:HA	5:A:305:CPS:H8	1.34	1.07
1:A:227:GLU:N	1:A:227:GLU:OE1	1.91	1.04
1:B:233:LEU:HB3	1:B:234:PRO:HD3	1.45	0.96
1:B:176:GLU:CD	1:B:177:ASN:H	1.75	0.90
1:B:210:THR:HG22	1:B:219:VAL:HG21	1.56	0.88
1:B:2:SER:HB2	1:B:4:ILE:HG22	1.59	0.82
1:B:225:LEU:O	1:B:228:ILE:HG22	1.81	0.81
1:A:120:ILE:HG12	1:A:196:MET:HE1	1.64	0.79
1:A:72:MET:CE	2:A:301:STR:H191	2.16	0.74
1:A:72:MET:HE1	2:A:301:STR:H62	1.69	0.74
1:B:210:THR:CG2	1:B:219:VAL:HG21	2.18	0.73
1:A:233:LEU:HB3	1:A:234:PRO:HD3	1.71	0.72
1:B:191:LYS:NZ	1:B:247:HIS:HB2	2.05	0.71
1:A:227:GLU:CD	1:A:227:GLU:H	1.94	0.70
1:B:120:ILE:HG13	1:B:196:MET:CE	2.21	0.70
1:A:72:MET:CE	2:A:301:STR:H62	2.20	0.70
1:B:34:LEU:HD13	2:B:301:STR:H122	1.74	0.69
1:A:72:MET:HE3	2:A:301:STR:H191	1.72	0.69
1:A:232:GLN:O	1:A:236:VAL:HG23	1.91	0.69
1:A:34:LEU:HB3	2:A:301:STR:H122	1.75	0.68
1:B:178:ASN:ND2	1:B:181:GLN:HG3	2.10	0.67
1:B:176:GLU:OE1	1:B:177:ASN:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HB3	2:B:301:STR:H122	1.77	0.66
1:A:184:GLN:O	1:A:188:GLN:HG2	1.95	0.66
1:B:42:LEU:O	1:B:46:VAL:HG23	1.96	0.65
1:B:149:GLU:OE1	1:B:149:GLU:N	2.24	0.65
1:B:211:PHE:HE1	1:B:226:VAL:HG13	1.63	0.64
1:A:43:VAL:O	1:A:46:VAL:HG23	1.98	0.64
1:B:211:PHE:CE1	1:B:226:VAL:HG13	2.32	0.64
1:A:120:ILE:HG12	1:A:196:MET:CE	2.28	0.63
1:A:177:ASN:HB3	1:A:181:GLN:HB2	1.79	0.63
1:B:176:GLU:CD	1:B:177:ASN:N	2.50	0.62
1:A:28:ASN:HB3	7:A:403:HOH:O	2.00	0.62
1:A:56:ARG:HH11	1:A:56:ARG:HB2	1.64	0.62
1:B:121:SER:O	1:B:124:PHE:HB2	2.00	0.62
1:A:176:GLU:HA	1:A:176:GLU:OE2	2.00	0.61
1:A:235:LYS:O	1:A:240:MET:HG3	1.99	0.61
1:A:2:SER:HB3	1:A:170:ARG:HH12	1.65	0.61
1:B:210:THR:HB	1:B:221:PHE:HZ	1.64	0.61
1:B:233:LEU:HB3	1:B:234:PRO:CD	2.28	0.61
1:B:133:GLU:OE1	1:B:175:LYS:HE2	2.01	0.60
1:B:211:PHE:HA	1:B:221:PHE:CE2	2.37	0.60
1:B:34:LEU:HB3	2:B:301:STR:C12	2.32	0.60
1:A:72:MET:HE1	2:A:301:STR:H191	1.84	0.59
1:A:225:LEU:O	1:A:228:ILE:HG22	2.03	0.59
1:A:71:TRP:O	1:A:75:MET:HG3	2.01	0.59
1:A:246:PHE:O	1:A:247:HIS:HB2	2.03	0.58
1:A:23:GLN:HG3	1:A:29:TYR:CE2	2.38	0.58
1:B:191:LYS:HZ3	1:B:247:HIS:HB2	1.66	0.58
1:B:122:GLN:HA	1:B:125:VAL:HG13	1.84	0.58
1:B:52:LEU:HD12	1:B:53:PRO:HD2	1.86	0.58
1:A:98:LEU:HD11	1:A:100:PHE:HE1	1.68	0.58
1:B:29:TYR:O	1:B:33:SER:OG	2.21	0.57
1:B:40:LYS:O	1:B:43:VAL:HG22	2.05	0.57
1:A:121:SER:O	1:A:124:PHE:HB2	2.05	0.57
1:B:120:ILE:HG13	1:B:196:MET:HE1	1.85	0.57
1:B:175:LYS:HG2	1:B:176:GLU:N	2.19	0.57
1:B:184:GLN:O	1:B:188:GLN:HG3	2.05	0.56
1:B:31:LEU:HD11	1:B:110:MET:HE2	1.86	0.56
1:A:193:LEU:O	1:A:196:MET:HB2	2.05	0.56
5:A:305:CPS:H11B	5:A:305:CPS:H10A	1.87	0.56
1:B:232:GLN:O	1:B:236:VAL:HG12	2.05	0.56
1:B:83:SER:HB2	1:B:121:SER:OG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:HIS:O	1:B:62:ASP:HB2	2.07	0.55
1:A:87:THR:HG21	1:A:91:MET:HB2	1.89	0.54
1:B:153:SER:O	1:B:156:SER:N	2.39	0.54
1:B:59:HIS:ND1	1:B:152:LYS:HD2	2.23	0.54
1:B:225:LEU:O	1:B:229:ILE:HG13	2.08	0.54
1:B:35:ASN:HD21	2:B:301:STR:H183	1.73	0.53
1:B:153:SER:O	1:B:155:ALA:N	2.41	0.53
1:A:224:MET:HG3	4:A:304:MES:H61	1.90	0.52
1:A:58:LEU:HD23	1:A:156:SER:HB2	1.91	0.52
1:A:72:MET:HE1	2:A:301:STR:C6	2.40	0.52
1:B:2:SER:HB2	1:B:170:ARG:HH12	1.73	0.52
1:B:34:LEU:CD1	2:B:301:STR:H122	2.38	0.52
5:A:305:CPS:H10A	5:A:305:CPS:C11	2.40	0.51
1:A:56:ARG:HH11	1:A:56:ARG:CB	2.24	0.51
1:B:209:TYR:HD1	5:B:303:CPS:HO2	1.56	0.51
1:B:99:ILE:N	7:B:401:HOH:O	2.37	0.51
1:B:62:ASP:OD1	1:B:151:LEU:HB3	2.10	0.51
1:A:52:LEU:HD23	1:A:53:PRO:HD2	1.94	0.50
1:A:92:LEU:HB2	1:A:100:PHE:HB2	1.94	0.50
1:A:131:GLN:O	1:A:135:LEU:HG	2.12	0.50
1:A:69:TYR:HB3	1:A:145:THR:CG2	2.41	0.50
1:A:42:LEU:O	1:A:46:VAL:HG22	2.12	0.50
1:A:209:TYR:CA	5:A:305:CPS:H8	2.24	0.50
1:A:63:GLN:O	1:A:67:ILE:HG13	2.11	0.49
1:B:92:LEU:HB2	1:B:100:PHE:HB2	1.94	0.49
1:A:123:GLU:OE1	1:A:126:ARG:HD3	2.12	0.49
1:B:115:GLN:O	1:B:119:GLN:HG2	2.12	0.49
1:B:196:MET:CE	1:B:199:LEU:HD23	2.42	0.49
1:B:193:LEU:O	1:B:196:MET:HB2	2.12	0.49
2:B:301:STR:H112	2:B:301:STR:H12	1.75	0.48
1:A:113:LEU:HD13	1:A:203:LEU:HD23	1.94	0.48
1:B:41:GLN:O	1:B:45:VAL:HG13	2.13	0.48
1:B:31:LEU:HG	2:B:301:STR:H213	1.96	0.48
1:B:35:ASN:ND2	2:B:301:STR:H183	2.29	0.48
1:B:191:LYS:HZ1	1:B:247:HIS:HB2	1.77	0.48
1:B:228:ILE:HG23	1:B:229:ILE:N	2.29	0.47
1:A:223:GLU:O	1:A:226:VAL:HB	2.14	0.47
1:A:60:LEU:O	1:A:60:LEU:HD23	2.13	0.47
1:A:110:MET:HE1	2:A:301:STR:H151	1.96	0.47
1:B:222:PRO:O	1:B:226:VAL:HG23	2.14	0.47
1:B:63:GLN:O	1:B:67:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:SER:O	1:A:218:SER:N	2.46	0.47
1:A:43:VAL:O	1:A:46:VAL:CG2	2.61	0.47
1:B:87:THR:O	1:B:90:GLN:HB2	2.15	0.47
1:A:69:TYR:HB3	1:A:145:THR:HG21	1.98	0.46
1:A:59:HIS:ND1	1:A:152:LYS:HD2	2.30	0.46
1:B:116:GLY:HA2	1:B:119:GLN:HG3	1.97	0.46
1:B:2:SER:CB	1:B:170:ARG:HH12	2.28	0.46
1:A:56:ARG:NH1	1:A:56:ARG:HB2	2.30	0.46
1:B:147:PRO:HA	1:B:240:MET:O	2.16	0.46
1:A:8:GLN:NE2	1:A:131:GLN:OE1	2.48	0.46
1:A:2:SER:HB2	1:A:5:SER:H	1.81	0.46
1:A:199:LEU:O	1:A:199:LEU:HD12	2.16	0.45
1:A:213:GLN:O	1:A:216:ALA:HB3	2.16	0.45
1:A:209:TYR:HE2	1:A:217:LEU:HD11	1.81	0.45
1:A:72:MET:HE1	2:A:301:STR:H8	1.98	0.45
1:B:11:GLU:OE1	1:B:11:GLU:HA	2.17	0.45
1:B:153:SER:O	1:B:154:GLN:C	2.54	0.45
1:B:184:GLN:HG3	1:B:185:ARG:N	2.31	0.45
1:B:187:TYR:O	1:B:191:LYS:HB2	2.17	0.45
4:B:302:MES:H81	4:B:302:MES:H31	1.62	0.45
1:B:2:SER:HB2	1:B:4:ILE:CG2	2.41	0.45
1:B:115:GLN:HA	1:B:115:GLN:OE1	2.17	0.44
1:B:186:PHE:CE2	1:B:190:THR:HG21	2.52	0.44
1:A:77:PHE:HD1	1:A:196:MET:HE3	1.83	0.44
1:A:228:ILE:HG23	1:A:229:ILE:N	2.33	0.44
1:A:217:LEU:HD23	1:A:217:LEU:HA	1.80	0.44
1:A:133:GLU:OE2	1:A:185:ARG:NH2	2.45	0.43
1:B:210:THR:HG22	1:B:219:VAL:CG2	2.39	0.43
1:A:178:ASN:OD1	1:A:181:GLN:HG3	2.19	0.43
1:B:245:LEU:N	1:B:245:LEU:HD23	2.33	0.43
5:A:305:CPS:H18	5:A:305:CPS:H11	1.70	0.43
1:B:213:GLN:HB2	1:B:217:LEU:CD1	2.48	0.43
1:A:209:TYR:CE2	1:A:217:LEU:HD11	2.54	0.43
1:B:225:LEU:O	1:B:228:ILE:CG2	2.58	0.43
1:B:126:ARG:HG2	1:B:126:ARG:HH11	1.84	0.43
1:B:210:THR:HA	1:B:217:LEU:CD1	2.49	0.43
1:B:4:ILE:HG23	1:B:5:SER:N	2.34	0.43
1:B:187:TYR:CZ	1:B:191:LYS:HG3	2.53	0.42
1:A:3:LEU:HD21	1:A:164:TYR:CE1	2.53	0.42
1:A:140:LEU:HD21	1:A:165:ILE:HG13	2.01	0.42
1:B:126:ARG:HG2	1:B:126:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:SER:C	1:B:155:ALA:N	2.73	0.42
5:A:305:CPS:C19	5:A:305:CPS:H10A	2.35	0.42
1:B:196:MET:HE1	1:B:199:LEU:HD23	2.01	0.42
1:A:72:MET:HE1	2:A:301:STR:C7	2.50	0.42
1:A:46:VAL:HG12	1:A:67:ILE:HD13	2.01	0.42
1:A:235:LYS:HA	1:A:240:MET:HE3	2.02	0.42
1:B:178:ASN:O	1:B:181:GLN:HB2	2.19	0.42
1:B:233:LEU:C	1:B:233:LEU:HD12	2.40	0.42
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.84	0.42
1:B:148:LYS:HE2	1:B:239:GLY:O	2.20	0.42
1:B:189:LEU:O	1:B:192:LEU:HB3	2.19	0.42
1:B:224:MET:HG3	4:B:302:MES:H22	2.02	0.41
1:A:64:MET:HG3	1:A:65:THR:N	2.35	0.41
1:B:59:HIS:O	1:B:62:ASP:N	2.52	0.41
1:A:110:MET:HB2	1:A:110:MET:HE2	1.75	0.41
1:A:41:GLN:O	1:A:45:VAL:HG23	2.20	0.41
1:A:154:GLN:O	1:A:155:ALA:C	2.58	0.41
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.82	0.41
1:B:245:LEU:N	1:B:245:LEU:CD2	2.84	0.41
1:B:188:GLN:HG3	1:B:188:GLN:H	1.72	0.41
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.93	0.41
1:B:49:ALA:O	1:B:52:LEU:HB3	2.20	0.41
1:B:105:MET:HE3	1:B:105:MET:HB2	1.97	0.41
1:B:167:GLU:OE1	1:B:170:ARG:HD3	2.20	0.41
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.75	0.41
1:B:139:ALA:O	1:B:142:LEU:HB3	2.20	0.41
1:B:3:LEU:HG	1:B:167:GLU:OE2	2.21	0.41
1:A:56:ARG:O	1:A:56:ARG:HG2	2.20	0.40
1:B:134:PHE:CZ	1:B:138:LYS:HD3	2.57	0.40
1:B:162:MET:O	1:B:165:ILE:HB	2.21	0.40
1:B:193:LEU:HA	1:B:193:LEU:HD23	1.91	0.40
1:A:105:MET:CE	1:A:114:CYS:HB3	2.51	0.40
1:B:93:TYR:CZ	1:B:96:PRO:HA	2.56	0.40
1:A:35:ASN:ND2	2:A:301:STR:H121	2.36	0.40
1:B:35:ASN:ND2	2:B:301:STR:H212	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/254 (98%)	240 (97%)	7 (3%)	1 (0%)	34	72
1	B	247/254 (97%)	242 (98%)	5 (2%)	0	100	100
All	All	495/508 (97%)	482 (97%)	12 (2%)	1 (0%)	47	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ALA

5.3.2 Protein sidechains

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	221/224 (99%)	204 (92%)	17 (8%)	13	42
1	B	220/224 (98%)	202 (92%)	18 (8%)	11	39
All	All	441/448 (98%)	406 (92%)	35 (8%)	12	41

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	2	SER
1	A	8	GLN
1	A	14	VAL
1	A	43	VAL

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Mol	Chain	Res	Type
1	A	46	VAL
1	A	52	LEU
1	A	56	ARG
1	A	60	LEU
1	A	64	MET
1	A	110	MET
1	A	115	GLN
1	A	195	SER
1	A	199	LEU
1	A	200	VAL
1	A	240	MET
1	A	247	HIS
1	B	3	LEU
1	B	14	VAL
1	B	26	THR
1	B	33	SER
1	B	39	GLU
1	B	44	SER
1	B	58	LEU
1	B	68	GLN
1	B	110	MET
1	B	119	GLN
1	B	175	LYS
1	B	178	ASN
1	B	179	SER
1	B	191	LYS
1	B	215	GLN
1	B	220	GLU
1	B	233	LEU
1	B	245	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	213	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 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
4	MES	A	304	-	12,12,12	2.30	1 (8%)	14,16,16	2.59	7 (50%)
3	GOL	A	302	-	5,5,5	0.38	0	5,5,5	0.27	0
2	STR	B	301	-	26,26,26	2.81	7 (26%)	42,42,42	3.07	15 (35%)
6	SO4	A	306	-	4,4,4	0.19	0	6,6,6	0.33	0
4	MES	B	302	-	12,12,12	2.21	1 (8%)	14,16,16	2.25	5 (35%)
3	GOL	A	303	-	5,5,5	0.54	0	5,5,5	0.76	0
5	CPS	B	303	-	28,28,45	2.09	10 (35%)	46,46,70	3.38	10 (21%)
2	STR	A	301	-	26,26,26	2.78	6 (23%)	42,42,42	2.97	15 (35%)
5	CPS	A	305	-	26,26,45	2.27	9 (34%)	40,43,70	4.49	16 (40%)

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
4	MES	A	304	-	-	6/6/14/14	0/1/1/1
3	GOL	A	302	-	-	0/4/4/4	-
2	STR	B	301	-	-	0/4/62/62	0/4/4/4
4	MES	B	302	-	-	6/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	303	-	-	1/4/4/4	-
5	CPS	B	303	-	-	0/4/69/90	0/4/4/4
2	STR	A	301	-	-	0/4/62/62	0/4/4/4
5	CPS	A	305	-	-	-	0/4/4/4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	STR	C4-C5	10.83	1.50	1.34
2	A	301	STR	C4-C5	10.31	1.49	1.34
4	A	304	MES	C8-S	-7.56	1.66	1.77
4	B	302	MES	C8-S	-7.24	1.67	1.77
5	B	303	CPS	C10-C5	-6.22	1.44	1.54
5	A	305	CPS	C10-C5	-6.00	1.44	1.54
2	A	301	STR	C18-C13	-4.92	1.45	1.54
2	B	301	STR	C18-C13	-4.87	1.45	1.54
5	A	305	CPS	C5-C9	-4.77	1.47	1.55
2	A	301	STR	C13-C17	-4.04	1.49	1.56
2	B	301	STR	C17-C20	3.74	1.57	1.51
5	B	303	CPS	C11-C2	-3.66	1.47	1.54
2	A	301	STR	C17-C20	3.60	1.57	1.51
2	B	301	STR	C13-C17	-3.31	1.50	1.56
5	A	305	CPS	O4-C4	-3.31	1.38	1.43
5	A	305	CPS	C11-C2	-3.26	1.48	1.54
5	B	303	CPS	C5-C9	-3.20	1.50	1.55
5	A	305	CPS	C20-C9	2.81	1.59	1.53
5	B	303	CPS	O4-C4	-2.80	1.39	1.43
5	A	305	CPS	C16-C17	2.63	1.57	1.52
5	A	305	CPS	C18-C19	-2.56	1.48	1.53
5	B	303	CPS	C18-C6	2.55	1.58	1.53
5	B	303	CPS	C16-C17	2.53	1.57	1.52
5	A	305	CPS	O3-C17	-2.52	1.38	1.43
2	A	301	STR	C13-C14	-2.50	1.50	1.55
5	B	303	CPS	C9-C20	2.43	1.60	1.54
5	A	305	CPS	C5-C6	-2.33	1.51	1.55
5	B	303	CPS	O3-C17	-2.33	1.38	1.43
2	A	301	STR	C8-C14	2.16	1.57	1.53
2	B	301	STR	C8-C14	2.14	1.57	1.53
2	B	301	STR	C4-C3	2.11	1.50	1.45
5	B	303	CPS	C18-C19	-2.08	1.49	1.53
2	B	301	STR	C13-C14	-2.05	1.51	1.55
5	B	303	CPS	C3-C19	2.03	1.57	1.53

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	305	CPS	C9-C5-C4	16.37	132.61	117.67
5	B	303	CPS	C10-C5-C4	-14.86	93.93	109.07
5	A	305	CPS	C10-C5-C4	-14.54	94.26	109.07
5	B	303	CPS	C9-C5-C4	11.99	128.61	117.67
2	B	301	STR	C12-C13-C17	10.50	128.93	116.10
2	B	301	STR	C18-C13-C12	-10.17	94.53	110.59
2	A	301	STR	C12-C13-C17	10.09	128.42	116.10
2	A	301	STR	C18-C13-C12	-9.37	95.80	110.59
5	A	305	CPS	C2-C19-C18	-7.82	103.43	111.82
5	A	305	CPS	C9-C5-C6	6.97	107.17	100.10
2	A	301	STR	C19-C10-C1	-6.01	99.93	109.43
5	A	305	CPS	C11-C2-C1	-5.79	98.92	108.26
5	A	305	CPS	C1-C2-C15	5.77	116.31	107.77
4	A	304	MES	C5-N4-C3	5.57	121.36	108.83
2	B	301	STR	C19-C10-C1	-5.09	101.38	109.43
5	B	303	CPS	C9-C5-C6	5.04	105.18	100.09
5	B	303	CPS	C11-C2-C1	-4.99	100.23	108.26
2	B	301	STR	C13-C17-C20	4.96	121.97	114.98
5	A	305	CPS	C7-C6-C5	4.92	108.38	103.55
4	B	302	MES	C5-N4-C3	4.85	119.75	108.83
2	A	301	STR	C5-C4-C3	-4.76	115.99	123.67
5	A	305	CPS	C19-C18-C17	-4.75	106.19	111.88
2	B	301	STR	C1-C10-C5	4.43	116.87	108.75
5	B	303	CPS	C6-C5-C4	4.39	111.49	107.40
4	B	302	MES	O1S-S-C8	4.33	112.13	106.92
5	B	303	CPS	C10-C5-C9	-4.33	104.44	111.21
5	A	305	CPS	C5-C6-C18	-4.22	109.34	114.74
2	B	301	STR	C5-C4-C3	-4.16	116.96	123.67
2	A	301	STR	C18-C13-C17	-4.02	103.73	110.24
2	A	301	STR	C13-C17-C20	3.94	120.53	114.98
5	A	305	CPS	C19-C18-C6	3.89	115.05	109.71
5	B	303	CPS	C1-C2-C15	3.83	113.44	107.77
4	A	304	MES	C6-C5-N4	-3.83	104.30	110.10
2	A	301	STR	C17-C13-C14	3.79	103.76	99.72
2	B	301	STR	C17-C13-C14	3.72	103.69	99.72
5	B	303	CPS	C19-C2-C15	3.69	113.77	108.58
4	A	304	MES	C7-N4-C5	3.64	120.55	111.23
2	A	301	STR	C1-C10-C5	3.36	114.90	108.75
4	A	304	MES	O3S-S-C8	3.29	111.09	105.77
5	A	305	CPS	C15-C14-C13	-3.06	108.26	112.76
2	A	301	STR	C12-C13-C14	3.03	111.98	107.27
2	A	301	STR	C14-C8-C9	3.02	113.13	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	STR	C14-C8-C9	3.02	113.13	109.09
5	A	305	CPS	O4-C4-C5	-2.91	106.12	111.03
5	A	305	CPS	C19-C2-C15	2.86	112.60	108.58
2	B	301	STR	C10-C9-C8	-2.81	108.52	112.73
2	B	301	STR	C18-C13-C17	-2.80	105.70	110.24
5	A	305	CPS	C3-C19-C18	2.76	114.92	110.88
2	B	301	STR	C12-C13-C14	2.74	111.52	107.27
5	A	305	CPS	C16-C15-C2	2.71	115.53	112.66
4	A	304	MES	C7-N4-C3	2.64	117.99	111.23
2	B	301	STR	C2-C1-C10	2.61	118.36	113.45
2	B	301	STR	C15-C14-C13	2.55	106.92	103.84
2	A	301	STR	C21-C20-C17	2.48	121.16	117.56
4	A	304	MES	C2-C3-N4	-2.44	106.41	110.10
4	B	302	MES	O2S-S-C8	2.38	109.78	106.92
4	A	304	MES	O1S-S-C8	2.37	109.77	106.92
5	B	303	CPS	C19-C18-C6	2.35	112.94	109.71
2	A	301	STR	C6-C5-C10	-2.30	112.52	116.77
4	B	302	MES	C7-N4-C5	2.30	117.11	111.23
5	B	303	CPS	C7-C6-C5	2.29	105.80	103.55
2	B	301	STR	C21-C20-C17	2.23	120.80	117.56
2	B	301	STR	C6-C5-C10	-2.19	112.73	116.77
2	A	301	STR	C2-C1-C10	2.14	117.47	113.45
2	A	301	STR	C16-C17-C13	-2.12	102.32	104.21
5	A	305	CPS	C20-C9-C8	-2.10	109.01	113.68
4	B	302	MES	C2-C3-N4	-2.09	106.94	110.10
2	A	301	STR	C10-C5-C4	-2.05	119.36	122.68

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	MES	C8-C7-N4-C5
4	A	304	MES	N4-C7-C8-S
4	A	304	MES	C7-C8-S-O1S
4	A	304	MES	C7-C8-S-O3S
4	B	302	MES	C8-C7-N4-C3
4	B	302	MES	C8-C7-N4-C5
4	B	302	MES	C7-C8-S-O1S
4	B	302	MES	C7-C8-S-O3S
4	B	302	MES	N4-C7-C8-S
4	A	304	MES	C7-C8-S-O2S
4	B	302	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
4	A	304	MES	C8-C7-N4-C3
3	A	303	GOL	O2-C2-C3-O3

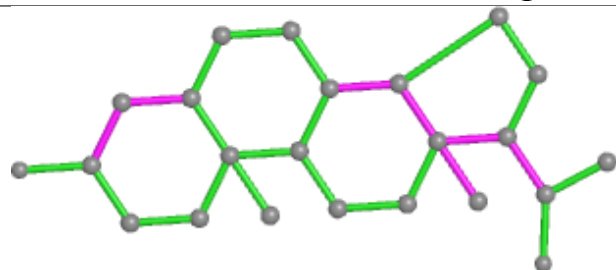
There are no ring outliers.

6 monomers are involved in 30 short contacts:

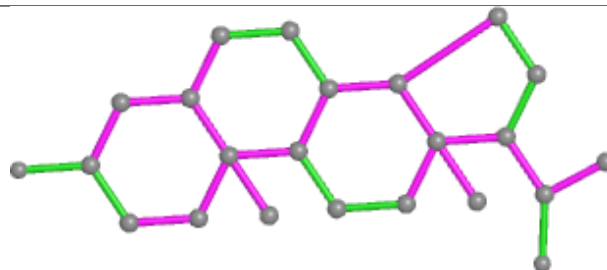
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	MES	1	0
2	B	301	STR	9	0
4	B	302	MES	2	0
5	B	303	CPS	1	0
2	A	301	STR	11	0
5	A	305	CPS	6	0

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.

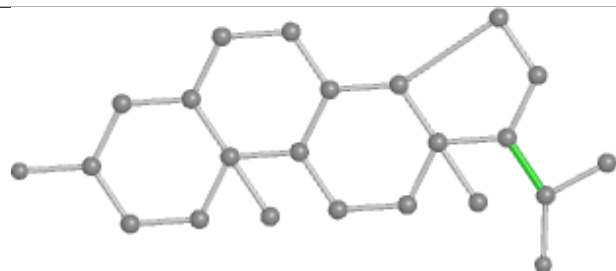
Ligand STR B 301



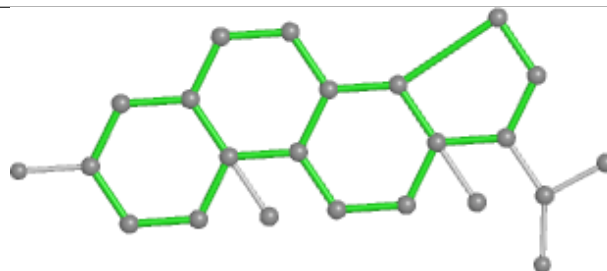
Bond lengths



Bond angles

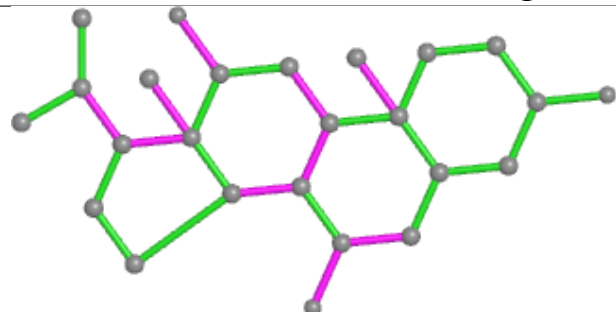


Torsions

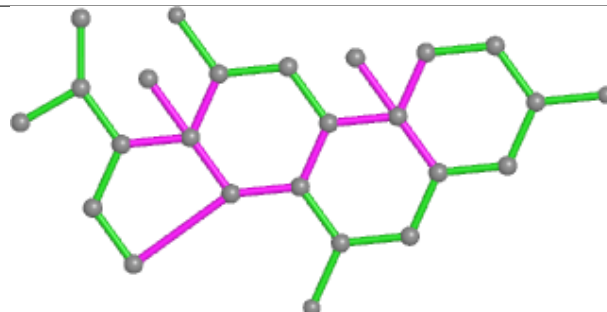


Rings

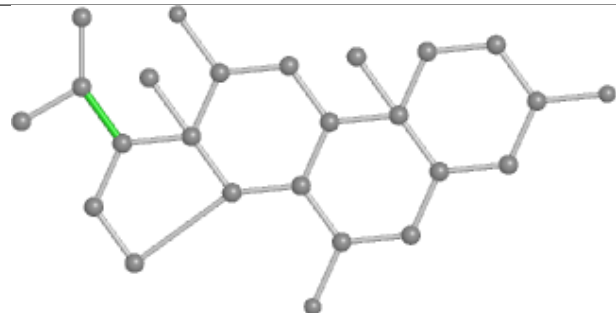
Ligand CPS B 303



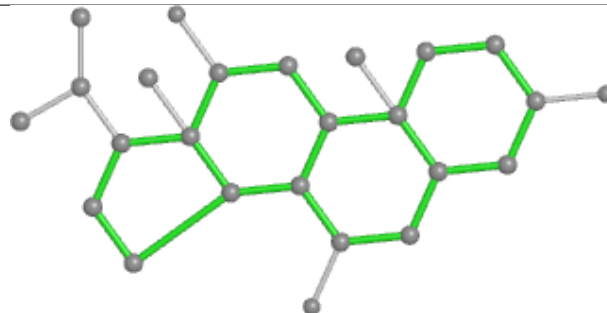
Bond lengths



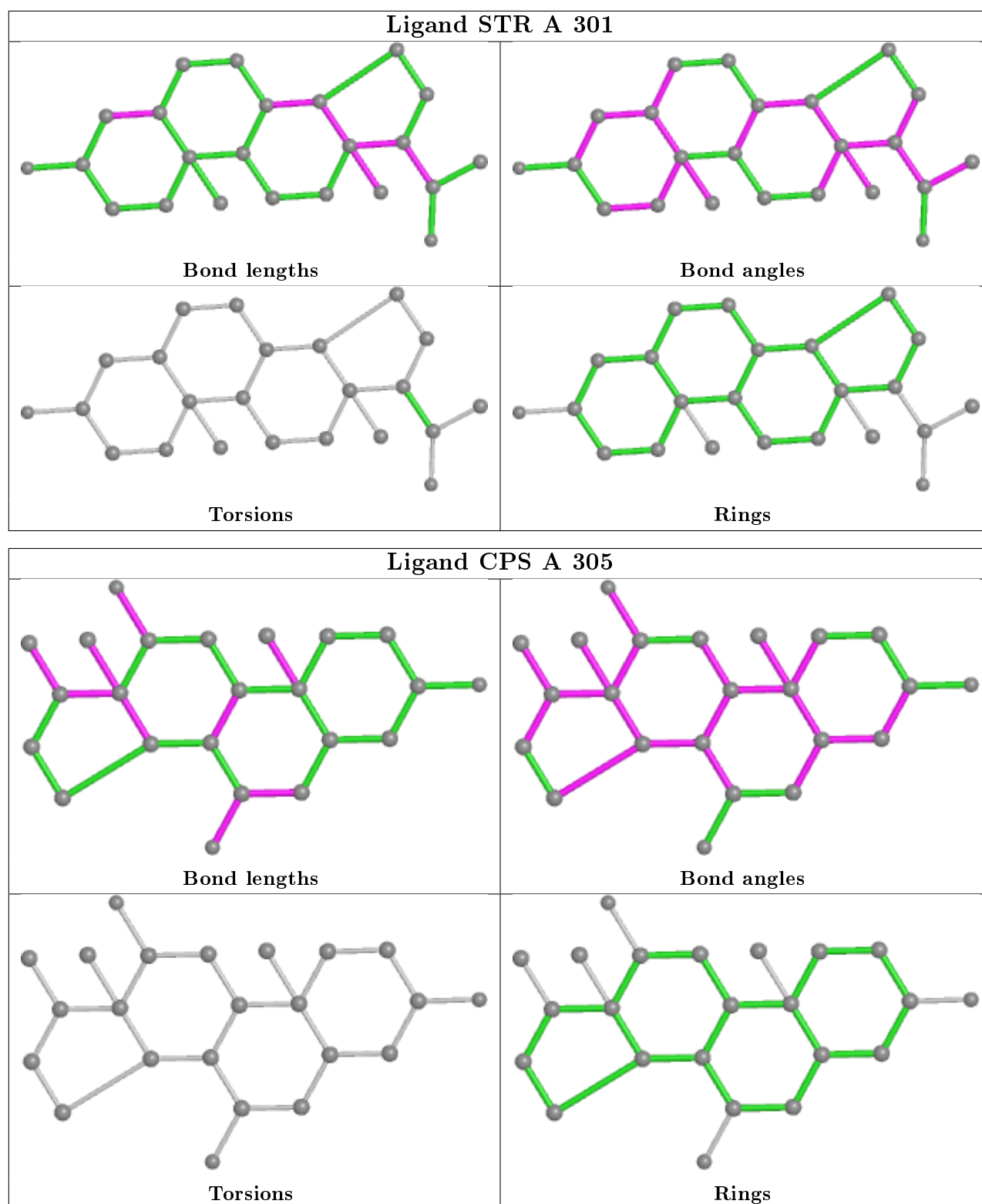
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	250/254 (98%)	-0.11	1 (0%) 92 79	42, 64, 88, 101	0
1	B	249/254 (98%)	-0.11	1 (0%) 92 79	42, 64, 90, 102	0
All	All	499/508 (98%)	-0.11	2 (0%) 92 79	42, 64, 89, 102	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	LYS	2.6
1	A	247	HIS	2.5

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, 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
3	GOL	A	303	6/6	0.70	0.25	65,72,89,90	0
4	MES	B	302	12/12	0.78	0.23	86,93,115,125	0
6	SO4	A	306	5/5	0.85	0.30	59,60,64,77	5

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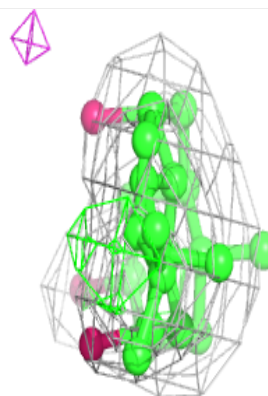
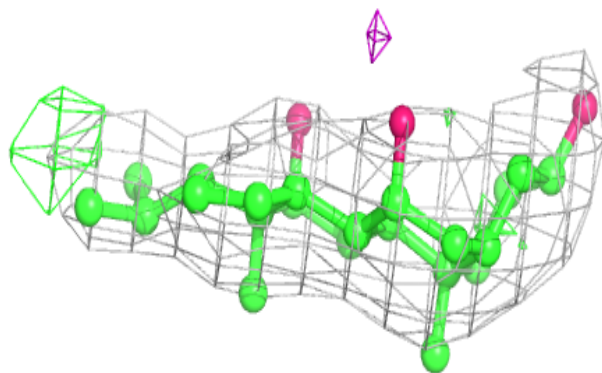
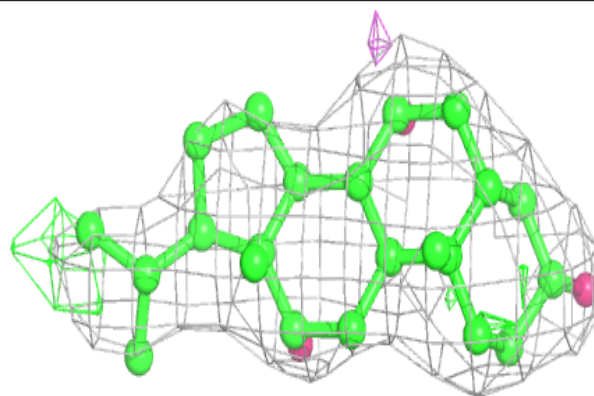
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	302	6/6	0.86	0.15	67,76,84,86	0
4	MES	A	304	12/12	0.87	0.23	81,88,120,124	0
5	CPS	B	303	25/42	0.89	0.33	79,88,100,104	0
5	CPS	A	305	23/42	0.91	0.23	77,92,102,106	0
2	STR	A	301	23/23	0.97	0.25	54,58,65,66	0
2	STR	B	301	23/23	0.97	0.22	51,56,61,62	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.

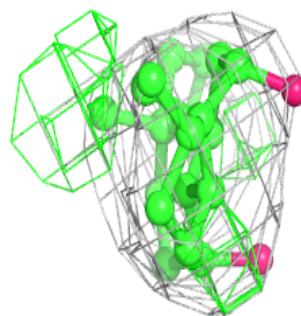
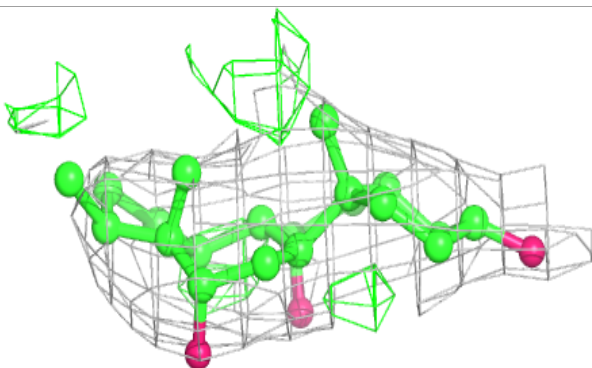
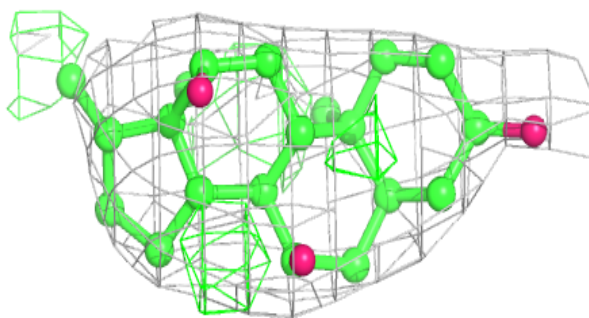
Electron density around CPS B 303:

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

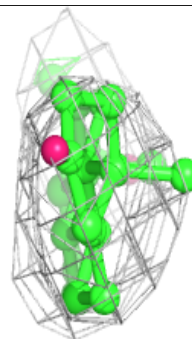
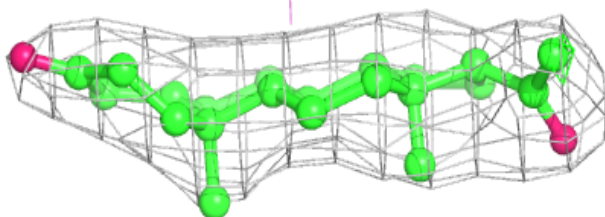
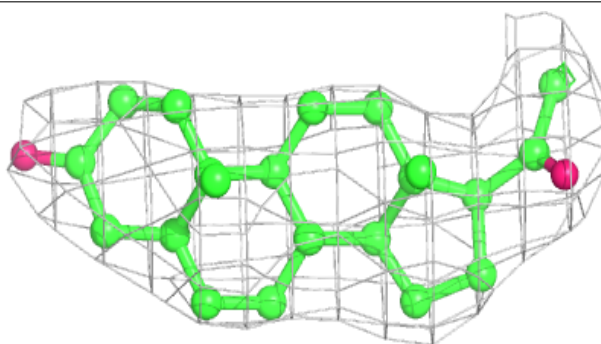


Electron density around CPS A 305:

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

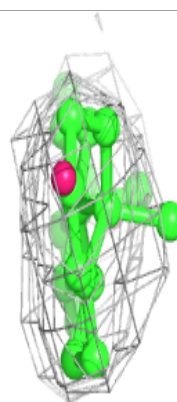
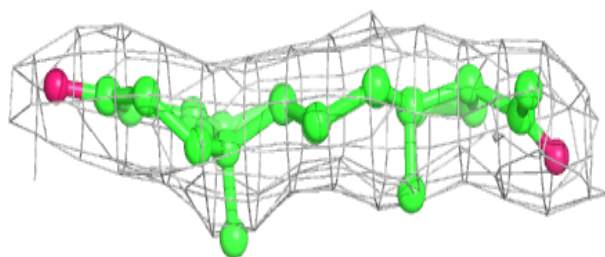
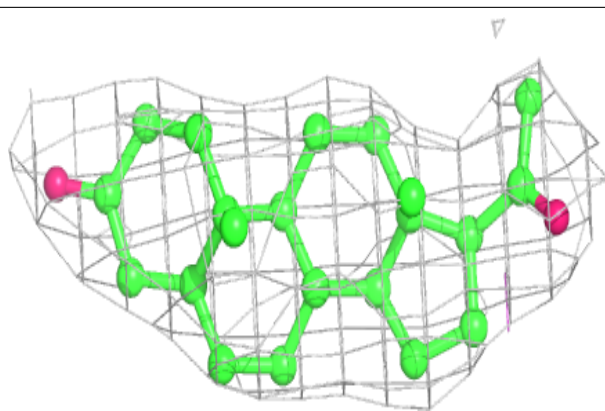
**Electron density around STR A 301:**

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



Electron density around STR B 301:

$2mF_o-DF_c$ (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.