Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:59 AM UTC

PDB ID	:	3WO2 / pdb_00003wo2
Title	:	Crystal structure of human interleukin-18
Authors	:	Tsutsumi, N.; Kimura, T.; Arita, K.; Ariyoshi, M.; Ohnishi, H.; Kondo, N.; Shirakawa, M.; Kato, Z.; Tochio, H.
Deposited on	:	2013-12-19
Resolution	:	2.33 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:

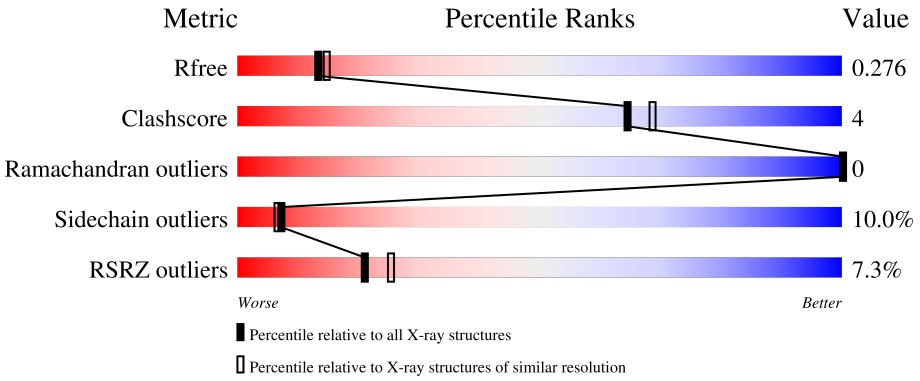
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	157	8% 79% 19% ·
1	B	157	6% 81% 18% ··
1	C	157	4% 80% 18% ·
1	D	157	10% 83% 16% ·

2 Entry composition

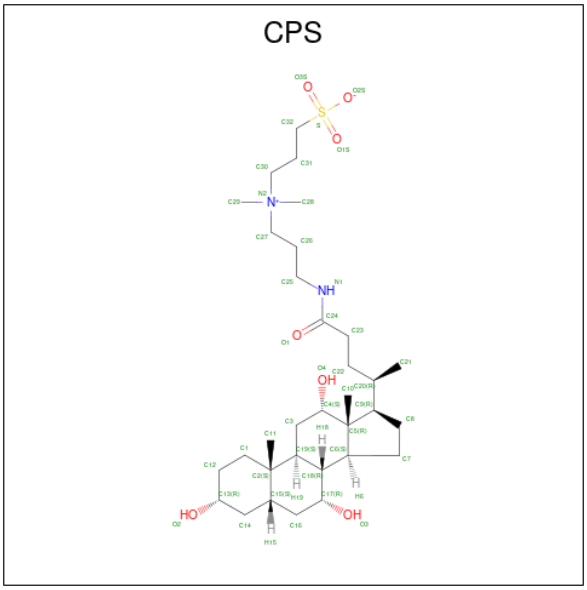
There are 4 unique types of molecules in this entry. The entry contains 5733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1257	793	208	246	10			
1	B	156	Total	C	N	O	S	0	0	0
			1233	779	204	240	10			
1	C	157	Total	C	N	O	S	0	0	0
			1266	796	211	250	9			
1	D	157	Total	C	N	O	S	0	1	0
			1266	801	211	244	10			

- Molecule 2 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (CCD ID: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			28	24	4			
2	A	1	Total	C	N	O	0	0
			30	25	1	4		

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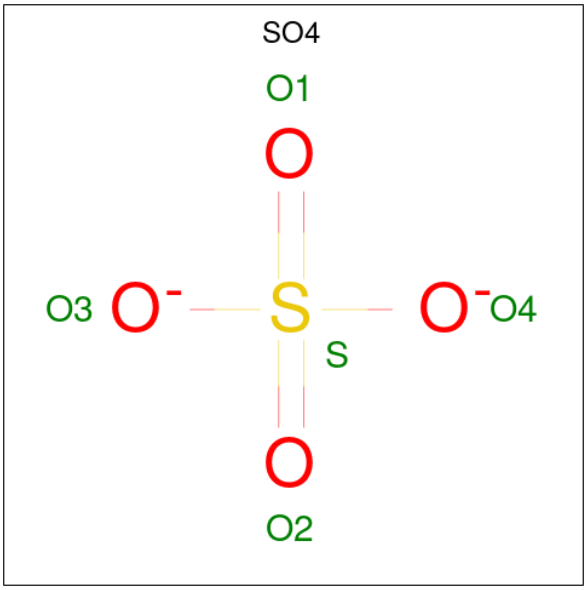
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 28 24 4	0	0
2	B	1	Total C N O 29 24 1 4	0	0
2	B	1	Total C O 23 20 3	0	0
2	B	1	Total C N O S 42 32 2 7 1	0	0
2	C	1	Total C O 26 23 3	0	0
2	C	1	Total C N O S 42 32 2 7 1	0	0
2	C	1	Total C O 26 23 3	0	0
2	D	1	Total C N O S 42 32 2 7 1	0	0
2	D	1	Total C O 23 20 3	0	0
2	D	1	Total C N O S 42 32 2 7 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

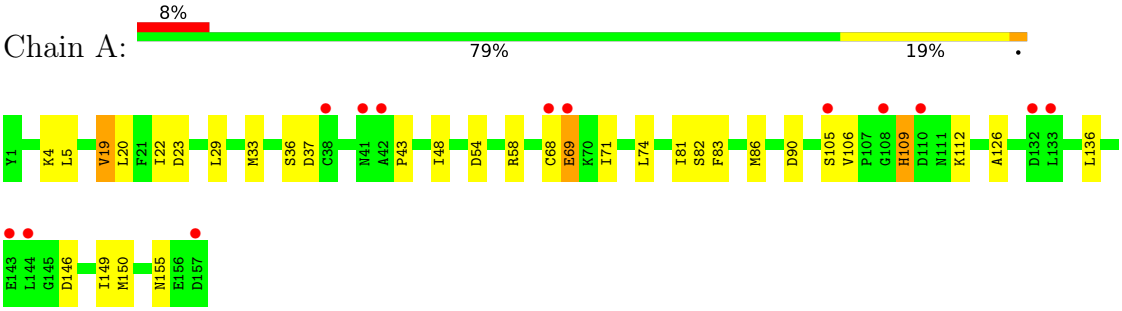
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	79	Total O 79 79	0	0
4	B	93	Total O 93 93	0	0
4	C	82	Total O 82 82	0	0
4	D	56	Total O 56 56	0	0

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.

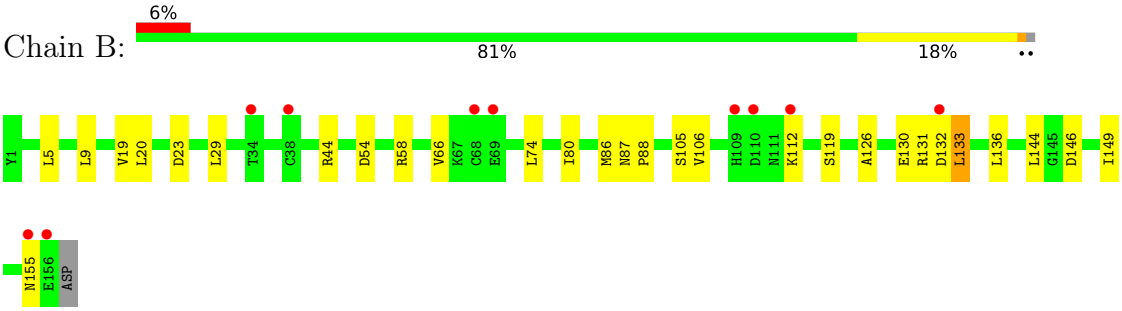
• Molecule 1: Interleukin-18

Chain A:



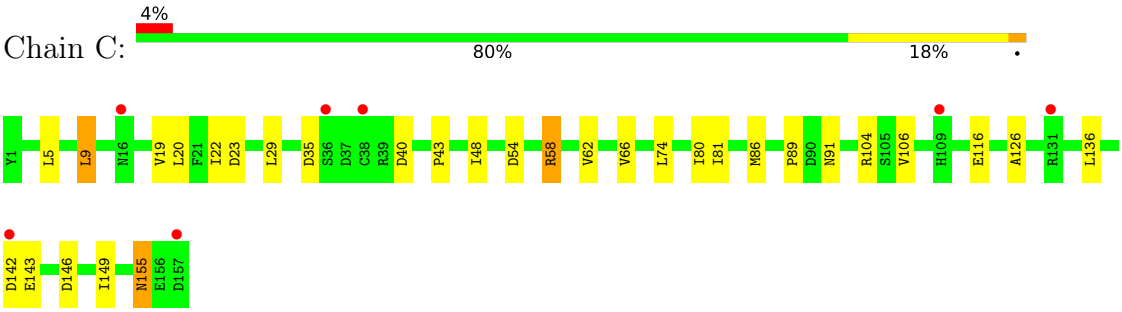
• Molecule 1: Interleukin-18

Chain B:



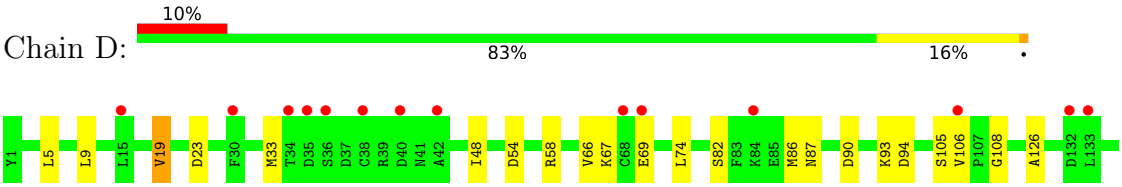
• Molecule 1: Interleukin-18

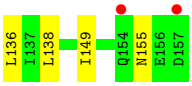
Chain C:



• Molecule 1: Interleukin-18

Chain D:




L136
I137
L138
I149
Q154
N155
E156
D157

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.15Å 79.51Å 73.46Å 90.00° 100.97° 90.00°	Depositor
Resolution (Å)	34.82 – 2.33 34.82 – 2.33	Depositor EDS
% Data completeness (in resolution range)	97.3 (34.82-2.33) 97.5 (34.82-2.33)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.218 , 0.271 0.225 , 0.276	Depositor DCC
R_{free} test set	1640 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5733	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CPS

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	0.77	0/1278	1.20	5/1714 (0.3%)
1	B	0.76	0/1254	1.20	5/1687 (0.3%)
1	C	0.74	0/1287	1.19	4/1726 (0.2%)
1	D	0.73	0/1290	1.18	5/1729 (0.3%)
All	All	0.75	0/5109	1.19	19/6856 (0.3%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	23	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	23	ASP	CA-CB-CG	6.94	119.54	112.60
1	D	23	ASP	CA-CB-CG	6.90	119.50	112.60
1	D	155	ASN	CA-C-N	6.25	129.64	120.82
1	D	155	ASN	C-N-CA	6.25	129.64	120.82
1	B	105	SER	CA-C-N	-5.94	118.31	122.59
1	B	105	SER	C-N-CA	-5.94	118.31	122.59
1	B	23	ASP	CA-CB-CG	5.91	118.51	112.60
1	D	94	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	37	ASP	CA-C-N	5.64	127.84	120.28
1	A	37	ASP	C-N-CA	5.64	127.84	120.28
1	C	155	ASN	CA-C-N	5.62	130.34	122.36
1	C	155	ASN	C-N-CA	5.62	130.34	122.36
1	C	54	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	54	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	54	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	146	ASP	CA-CB-CG	5.24	117.84	112.60
1	D	54	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	146	ASP	CA-CB-CG	5.00	117.60	112.60

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	1257	0	1233	12	0
1	B	1233	0	1194	7	0
1	C	1266	0	1241	12	0
1	D	1266	0	1255	8	0
2	A	86	0	116	5	0
2	B	94	0	128	2	0
2	C	94	0	132	7	0
2	D	107	0	147	6	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	79	0	0	0	0
4	B	93	0	0	0	0
4	C	82	0	0	0	0
4	D	56	0	0	0	0
All	All	5733	0	5446	42	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 4.

All (42) 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:D:87:ASN:HB3	2:D:203:CPS:H22A	1.68	0.74
1:D:48:ILE:HD11	2:D:201:CPS:H14A	1.74	0.68
1:A:48:ILE:HD11	2:A:201:CPS:H14A	1.77	0.66
1:A:82:SER:HB3	1:C:80:ILE:HD13	1.77	0.65
1:B:80:ILE:HD13	1:D:82:SER:HB3	1.83	0.59
1:C:58:ARG:O	1:C:104:ARG:NH1	2.35	0.59
1:A:109:HIS:HB2	1:A:112:LYS:HE3	1.87	0.56
1:A:22:ILE:HD11	1:A:83:PHE:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ASP:H	2:D:203:CPS:H32A	1.72	0.54
1:B:130:GLU:O	1:B:131:ARG:HG3	2.09	0.53
1:A:43:PRO:HG3	2:A:201:CPS:H8	1.93	0.51
1:D:87:ASN:HB2	2:D:203:CPS:H272	1.92	0.51
2:A:201:CPS:H13	2:A:203:CPS:H7	1.92	0.51
1:B:29:LEU:HD21	1:B:133:LEU:HG	1.93	0.50
1:C:89:PRO:HA	2:C:202:CPS:H25A	1.93	0.49
1:A:71:ILE:HD11	2:A:201:CPS:O2	2.14	0.48
1:C:104:ARG:NH2	1:C:116:GLU:OE1	2.46	0.48
1:B:87:ASN:HD21	2:B:203:CPS:H272	1.80	0.47
1:C:48:ILE:HD11	2:C:203:CPS:H14A	1.97	0.46
1:C:91:ASN:HB2	2:C:202:CPS:H32A	1.96	0.46
1:D:106:VAL:HG12	1:D:108:GLY:H	1.80	0.46
1:A:19:VAL:HG13	1:A:33:MET:HB2	1.98	0.45
1:D:19:VAL:HG13	1:D:33:MET:HB2	1.99	0.45
1:A:69:GLU:H	1:A:69:GLU:HG2	1.58	0.45
2:C:201:CPS:H21A	2:C:201:CPS:H10B	1.98	0.45
1:A:106:VAL:HG11	1:A:150:MET:HE2	1.99	0.44
1:C:126:ALA:HB2	1:C:149:ILE:HG22	1.99	0.44
1:C:74:LEU:HD11	1:C:81:ILE:HG23	2.00	0.43
1:A:126:ALA:HB2	1:A:149:ILE:HG22	2.01	0.43
1:C:9:LEU:HB3	2:C:201:CPS:H14	2.01	0.43
1:B:126:ALA:HB2	1:B:149:ILE:HG22	2.00	0.43
1:A:4:LYS:NZ	1:A:90:ASP:OD1	2.51	0.42
2:D:202:CPS:H3	2:D:202:CPS:H1	1.93	0.42
1:B:131:ARG:HE	1:B:132:ASP:H	1.66	0.42
1:B:88:PRO:HD2	2:B:203:CPS:H21A	2.01	0.42
1:C:35:ASP:HB3	2:C:201:CPS:H22A	2.00	0.42
1:C:43:PRO:HG3	2:C:203:CPS:H8	2.01	0.42
2:D:201:CPS:H28B	2:D:201:CPS:H262	1.90	0.42
2:A:203:CPS:H21A	2:A:203:CPS:O4	2.20	0.41
1:D:126:ALA:HB2	1:D:149:ILE:HG22	2.02	0.41
1:A:74:LEU:HD11	1:A:81:ILE:HG23	2.03	0.41
1:C:143:GLU:HG3	1:C:146:ASP:HB2	2.03	0.40

There are no symmetry-related clashes.

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	155/157 (99%)	147 (95%)	8 (5%)	0	100	100
1	B	154/157 (98%)	146 (95%)	8 (5%)	0	100	100
1	C	155/157 (99%)	147 (95%)	8 (5%)	0	100	100
1	D	156/157 (99%)	148 (95%)	8 (5%)	0	100	100
All	All	620/628 (99%)	588 (95%)	32 (5%)	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	143/148 (97%)	130 (91%)	13 (9%)	9	9
1	B	138/148 (93%)	122 (88%)	16 (12%)	5	4
1	C	145/148 (98%)	130 (90%)	15 (10%)	7	6
1	D	144/148 (97%)	131 (91%)	13 (9%)	9	9
All	All	570/592 (96%)	513 (90%)	57 (10%)	7	6

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	19	VAL

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Mol	Chain	Res	Type
1	A	20	LEU
1	A	29	LEU
1	A	36	SER
1	A	58	ARG
1	A	68	CYS
1	A	69	GLU
1	A	86	MET
1	A	105	SER
1	A	109	HIS
1	A	136	LEU
1	A	155	ASN
1	B	5	LEU
1	B	9	LEU
1	B	19	VAL
1	B	20	LEU
1	B	44	ARG
1	B	58	ARG
1	B	66	VAL
1	B	74	LEU
1	B	86	MET
1	B	106	VAL
1	B	112	LYS
1	B	119	SER
1	B	133	LEU
1	B	136	LEU
1	B	144	LEU
1	B	155	ASN
1	C	5	LEU
1	C	9	LEU
1	C	19	VAL
1	C	20	LEU
1	C	22	ILE
1	C	29	LEU
1	C	40	ASP
1	C	58	ARG
1	C	62	VAL
1	C	66	VAL
1	C	86	MET
1	C	106	VAL
1	C	136	LEU
1	C	142	ASP
1	C	155	ASN

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Mol	Chain	Res	Type
1	D	5	LEU
1	D	9	LEU
1	D	19	VAL
1	D	58	ARG
1	D	66	VAL
1	D	67	LYS
1	D	69	GLU
1	D	74	LEU
1	D	86	MET
1	D	93	LYS
1	D	105	SER
1	D	136	LEU
1	D	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	87	ASN
1	B	87	ASN
1	C	24	GLN
1	D	78	ASN
1	D	154	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CPS	B	201	-	32,32,45	0.62	0	51,51,70	2.05	17 (33%)
3	SO4	B	204	-	4,4,4	0.25	0	6,6,6	0.07	0
2	CPS	A	202	-	33,33,45	0.61	0	52,52,70	1.99	18 (34%)
3	SO4	A	204	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	C	204	-	4,4,4	0.24	0	6,6,6	0.08	0
2	CPS	B	203	-	45,45,45	1.29	1 (2%)	70,70,70	1.82	23 (32%)
2	CPS	C	202	-	45,45,45	1.31	1 (2%)	70,70,70	1.82	19 (27%)
2	CPS	D	202	-	26,26,45	0.60	0	42,43,70	2.02	17 (40%)
2	CPS	D	201	-	45,45,45	1.27	1 (2%)	70,70,70	1.85	16 (22%)
3	SO4	A	205	-	4,4,4	0.24	0	6,6,6	0.12	0
2	CPS	A	201	-	30,31,45	0.58	0	49,49,70	1.73	12 (24%)
2	CPS	C	203	-	29,29,45	0.60	0	47,47,70	1.94	14 (29%)
2	CPS	C	201	-	29,29,45	0.48	0	47,47,70	2.36	19 (40%)
2	CPS	A	203	-	30,31,45	0.56	0	49,49,70	3.53	30 (61%)
2	CPS	B	202	-	26,26,45	0.65	0	42,43,70	1.92	15 (35%)
2	CPS	D	203	-	45,45,45	1.27	1 (2%)	70,70,70	1.74	18 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPS	B	201	-	-	1/9/74/90	0/4/4/4
2	CPS	A	202	-	-	2/11/76/90	0/4/4/4
2	CPS	B	203	-	-	9/25/90/90	0/4/4/4
2	CPS	C	202	-	-	14/25/90/90	0/4/4/4
2	CPS	D	202	-	-	-	0/4/4/4
2	CPS	D	201	-	-	17/25/90/90	0/4/4/4
2	CPS	A	201	-	-	5/8/73/90	0/4/4/4
2	CPS	C	203	-	-	2/6/71/90	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPS	C	201	-	-	4/6/71/90	0/4/4/4
2	CPS	A	203	-	-	4/8/73/90	0/4/4/4
2	CPS	B	202	-	-	-	0/4/4/4
2	CPS	D	203	-	-	18/25/90/90	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	202	CPS	C32-S	-7.42	1.67	1.77
2	D	201	CPS	C32-S	-7.23	1.67	1.77
2	B	203	CPS	C32-S	-7.22	1.67	1.77
2	D	203	CPS	C32-S	-7.12	1.67	1.77

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	203	CPS	C9-C5-C6	-12.30	87.77	100.11
2	A	203	CPS	C9-C5-C4	7.50	124.42	117.67
2	A	203	CPS	C16-C15-C2	7.17	120.30	112.66
2	C	201	CPS	C16-C15-C2	6.87	119.97	112.66
2	A	203	CPS	C5-C9-C20	6.38	127.21	119.48
2	A	203	CPS	C3-C4-C5	5.90	117.27	111.26
2	C	203	CPS	C7-C6-C5	5.37	108.75	103.54
2	C	202	CPS	C7-C6-C5	5.35	108.73	103.54
2	B	201	CPS	C14-C15-C2	5.27	118.27	112.66
2	A	203	CPS	C21-C20-C22	-5.14	102.38	110.34
2	A	202	CPS	C7-C6-C5	4.93	108.32	103.54
2	B	201	CPS	C7-C6-C5	4.90	108.29	103.54
2	C	201	CPS	C7-C6-C5	4.72	108.12	103.54
2	C	202	CPS	C14-C15-C2	4.69	117.65	112.66
2	D	201	CPS	C7-C6-C5	4.65	108.05	103.54
2	B	202	CPS	C14-C15-C2	4.65	117.61	112.66
2	D	203	CPS	C7-C6-C5	4.63	108.03	103.54
2	A	203	CPS	C14-C15-C2	4.54	117.49	112.66
2	C	201	CPS	C19-C2-C15	4.51	114.78	108.51
2	A	202	CPS	C14-C15-C2	4.51	117.46	112.66
2	D	201	CPS	C8-C9-C20	4.48	118.95	112.18
2	A	201	CPS	C7-C6-C5	4.45	107.85	103.54
2	B	203	CPS	C7-C6-C5	4.44	107.84	103.54
2	B	202	CPS	C7-C6-C5	4.40	107.81	103.54
2	B	203	CPS	C14-C15-C2	4.40	117.34	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	202	CPS	C7-C6-C5	4.37	107.78	103.54
2	B	201	CPS	C5-C9-C20	4.36	124.77	119.48
2	B	203	CPS	C5-C9-C20	4.34	124.74	119.48
2	A	203	CPS	C7-C6-C5	4.23	107.64	103.54
2	C	203	CPS	C3-C19-C18	4.18	117.08	110.89
2	B	203	CPS	C21-C20-C9	4.18	119.15	112.88
2	D	202	CPS	C14-C15-C2	4.16	117.09	112.66
2	D	201	CPS	C8-C9-C5	4.08	107.50	103.54
2	A	203	CPS	C3-C19-C2	4.06	117.82	113.70
2	C	201	CPS	C21-C20-C9	4.04	118.94	112.88
2	D	203	CPS	C14-C15-C2	3.99	116.91	112.66
2	D	201	CPS	C21-C20-C22	3.99	116.51	110.34
2	A	202	CPS	C5-C9-C20	3.98	124.31	119.48
2	B	201	CPS	C21-C20-C9	3.96	118.83	112.88
2	C	201	CPS	C5-C9-C20	3.96	124.28	119.48
2	D	202	CPS	C16-C15-C2	3.95	116.87	112.66
2	C	201	CPS	C1-C2-C19	-3.94	105.22	111.34
2	C	202	CPS	C8-C9-C5	3.94	107.36	103.54
2	C	201	CPS	C8-C9-C5	3.89	107.31	103.54
2	D	201	CPS	C3-C19-C18	3.84	116.58	110.89
2	C	201	CPS	C9-C5-C6	-3.70	96.40	100.11
2	A	202	CPS	C8-C9-C5	3.67	107.10	103.54
2	C	203	CPS	C5-C9-C20	3.63	123.88	119.48
2	C	203	CPS	C3-C19-C2	3.62	117.38	113.70
2	B	202	CPS	C3-C19-C18	3.62	116.25	110.89
2	A	202	CPS	C3-C4-C5	3.58	114.91	111.26
2	A	201	CPS	C14-C15-C2	3.55	116.44	112.66
2	B	203	CPS	C8-C9-C5	3.53	106.96	103.54
2	A	203	CPS	C7-C6-C18	3.52	123.19	118.36
2	D	202	CPS	C1-C2-C15	3.52	112.80	107.75
2	D	203	CPS	C8-C9-C5	3.51	106.95	103.54
2	B	201	CPS	C2-C19-C18	3.50	115.74	111.84
2	D	201	CPS	C16-C15-C2	3.48	116.37	112.66
2	A	203	CPS	C1-C2-C19	-3.46	105.97	111.34
2	A	203	CPS	C2-C19-C18	3.45	115.68	111.84
2	A	203	CPS	C21-C20-C9	3.44	118.05	112.88
2	D	201	CPS	C22-C20-C9	3.44	117.46	110.33
2	B	201	CPS	C15-C14-C13	3.43	117.89	112.71
2	B	202	CPS	C1-C2-C15	3.43	112.67	107.75
2	A	201	CPS	C3-C19-C18	3.42	115.96	110.89
2	A	203	CPS	C8-C7-C6	-3.37	98.55	105.14
2	D	203	CPS	C2-C19-C18	3.37	115.59	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	202	CPS	C3-C4-C5	3.33	114.65	111.26
2	A	203	CPS	C1-C2-C15	3.33	112.52	107.75
2	A	202	CPS	C2-C19-C18	3.31	115.53	111.84
2	A	203	CPS	C12-C1-C2	3.29	118.29	112.74
2	B	202	CPS	C16-C15-C2	3.27	116.14	112.66
2	A	203	CPS	C19-C2-C15	3.27	113.05	108.51
2	D	203	CPS	C16-C17-C18	3.25	115.05	111.50
2	A	203	CPS	O4-C4-C5	3.24	116.50	111.02
2	A	203	CPS	C19-C18-C17	-3.22	107.80	111.86
2	D	201	CPS	O1S-S-C32	3.21	111.58	106.73
2	C	201	CPS	C2-C19-C18	3.21	115.41	111.84
2	D	202	CPS	C11-C2-C1	-3.18	103.25	108.31
2	A	202	CPS	C9-C5-C6	-3.18	96.92	100.11
2	B	203	CPS	C2-C19-C18	3.16	115.36	111.84
2	D	202	CPS	C12-C1-C2	3.10	117.97	112.74
2	B	201	CPS	C6-C18-C17	3.08	115.93	111.85
2	A	202	CPS	C16-C15-C2	3.05	115.91	112.66
2	C	203	CPS	C16-C15-C2	3.05	115.90	112.66
2	B	203	CPS	C9-C5-C4	-3.02	114.95	117.67
2	A	203	CPS	C8-C9-C20	3.01	116.74	112.18
2	C	203	CPS	C8-C9-C5	3.00	106.45	103.54
2	C	201	CPS	C3-C19-C18	3.00	115.33	110.89
2	C	202	CPS	C15-C14-C13	2.96	117.18	112.71
2	D	201	CPS	C1-C2-C15	2.96	112.00	107.75
2	D	201	CPS	C11-C2-C1	-2.95	103.61	108.31
2	A	202	CPS	C21-C20-C9	2.94	117.30	112.88
2	D	201	CPS	C14-C15-C2	2.92	115.77	112.66
2	C	202	CPS	C21-C20-C22	-2.91	105.84	110.34
2	A	201	CPS	C6-C18-C17	2.88	115.67	111.85
2	C	203	CPS	C11-C2-C1	-2.87	103.75	108.31
2	B	201	CPS	C16-C15-C2	2.87	115.71	112.66
2	B	203	CPS	C3-C19-C18	2.85	115.11	110.89
2	C	202	CPS	C2-C19-C18	2.83	114.99	111.84
2	C	202	CPS	C5-C9-C20	2.83	122.91	119.48
2	B	203	CPS	C1-C2-C15	2.82	111.79	107.75
2	D	202	CPS	C3-C19-C18	2.79	115.03	110.89
2	B	201	CPS	C19-C2-C15	2.79	112.39	108.51
2	C	202	CPS	C14-C13-C12	2.76	113.99	110.62
2	B	201	CPS	C8-C9-C5	2.76	106.21	103.54
2	D	203	CPS	O2S-S-C32	2.75	111.38	106.00
2	A	203	CPS	C15-C16-C17	2.75	117.67	114.40
2	C	202	CPS	C9-C5-C6	-2.74	97.36	100.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	202	CPS	C3-C19-C2	2.74	116.48	113.70
2	C	203	CPS	C21-C20-C9	2.73	116.98	112.88
2	A	202	CPS	C11-C2-C1	-2.71	103.99	108.31
2	C	203	CPS	C14-C15-C2	2.69	115.53	112.66
2	B	203	CPS	O3S-S-C32	2.68	110.78	106.73
2	A	202	CPS	C3-C19-C2	2.68	116.42	113.70
2	D	203	CPS	C15-C14-C13	2.68	116.74	112.71
2	C	202	CPS	C3-C19-C2	2.66	116.41	113.70
2	B	201	CPS	C3-C4-C5	2.66	113.97	111.26
2	D	201	CPS	C6-C18-C17	2.65	115.37	111.85
2	A	203	CPS	C22-C20-C9	2.65	115.81	110.33
2	A	201	CPS	C11-C2-C1	-2.64	104.11	108.31
2	D	203	CPS	C3-C19-C2	2.62	116.36	113.70
2	D	203	CPS	C8-C9-C20	2.60	116.12	112.18
2	A	201	CPS	C16-C15-C2	2.60	115.43	112.66
2	C	202	CPS	C3-C19-C18	2.58	114.71	110.89
2	D	202	CPS	C10-C5-C6	2.55	115.20	111.20
2	D	202	CPS	C2-C19-C18	2.55	114.68	111.84
2	D	202	CPS	C1-C12-C13	2.54	113.85	110.48
2	A	203	CPS	C23-C22-C20	2.54	119.74	114.58
2	A	203	CPS	C3-C19-C18	2.54	114.65	110.89
2	C	202	CPS	O1S-S-C32	2.53	110.56	106.73
2	B	202	CPS	C11-C2-C1	-2.53	104.28	108.31
2	D	203	CPS	C3-C19-C18	2.53	114.64	110.89
2	C	201	CPS	C14-C15-C2	2.52	115.35	112.66
2	C	201	CPS	C12-C1-C2	2.52	116.99	112.74
2	D	203	CPS	C22-C20-C9	2.51	115.54	110.33
2	A	202	CPS	C19-C2-C15	2.49	111.97	108.51
2	C	202	CPS	C11-C2-C1	-2.48	104.36	108.31
2	B	202	CPS	C15-C14-C13	2.45	116.40	112.71
2	A	202	CPS	C16-C17-C18	2.44	114.17	111.50
2	D	202	CPS	C6-C5-C9	-2.43	97.67	100.12
2	B	202	CPS	C6-C18-C17	2.41	115.05	111.85
2	C	203	CPS	C1-C2-C15	2.40	111.19	107.75
2	C	201	CPS	C15-C14-C13	2.40	116.33	112.71
2	D	202	CPS	C11-C2-C15	-2.40	106.43	110.44
2	B	203	CPS	C21-C20-C22	2.40	114.05	110.34
2	B	203	CPS	C9-C5-C6	-2.39	97.71	100.11
2	A	202	CPS	C22-C20-C9	2.39	115.29	110.33
2	D	201	CPS	C12-C1-C2	2.38	116.76	112.74
2	C	203	CPS	C12-C1-C2	2.38	116.75	112.74
2	C	202	CPS	C5-C6-C18	2.37	117.72	114.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201	CPS	C3-C19-C18	2.36	114.39	110.89
2	D	202	CPS	C3-C4-C5	2.35	113.65	111.26
2	B	203	CPS	C3-C19-C2	2.34	116.08	113.70
2	D	203	CPS	C11-C2-C1	-2.33	104.60	108.31
2	C	202	CPS	O3S-S-C32	2.32	110.23	106.73
2	C	201	CPS	C1-C2-C15	2.31	111.06	107.75
2	D	203	CPS	C9-C5-C6	-2.30	97.80	100.11
2	A	202	CPS	C12-C1-C2	2.30	116.62	112.74
2	B	202	CPS	C8-C9-C5	2.29	108.02	103.30
2	B	202	CPS	C2-C19-C18	2.28	114.39	111.84
2	C	202	CPS	C16-C15-C2	2.28	115.09	112.66
2	B	203	CPS	C16-C17-C18	2.28	113.99	111.50
2	B	203	CPS	C6-C18-C17	2.27	114.86	111.85
2	A	201	CPS	C10-C5-C6	2.27	114.76	111.20
2	C	201	CPS	C11-C2-C15	-2.27	106.65	110.44
2	C	202	CPS	C16-C17-C18	2.26	113.97	111.50
2	A	203	CPS	C10-C5-C6	2.24	114.72	111.20
2	B	203	CPS	C16-C15-C2	2.24	115.05	112.66
2	A	203	CPS	C10-C5-C4	-2.23	106.82	109.06
2	A	202	CPS	C3-C19-C18	2.23	114.19	110.89
2	B	202	CPS	C9-C5-C4	-2.23	115.66	117.67
2	B	203	CPS	C12-C1-C2	2.22	116.49	112.74
2	D	201	CPS	C25-N1-C24	2.22	126.95	122.82
2	C	203	CPS	C10-C5-C6	2.21	114.66	111.20
2	B	201	CPS	C16-C17-C18	2.20	113.90	111.50
2	A	201	CPS	C15-C14-C13	2.19	116.02	112.71
2	A	203	CPS	C16-C15-C14	-2.18	108.73	111.23
2	B	202	CPS	C10-C5-C6	2.18	114.62	111.20
2	D	203	CPS	C3-C4-C5	2.18	113.48	111.26
2	C	201	CPS	C19-C18-C17	-2.18	109.12	111.86
2	B	201	CPS	C16-C15-C14	-2.17	108.74	111.23
2	C	203	CPS	C5-C6-C18	2.17	117.47	114.72
2	B	203	CPS	C7-C6-C18	2.17	121.33	118.36
2	A	201	CPS	C22-C20-C9	2.15	114.79	110.33
2	B	202	CPS	C7-C6-C18	2.15	121.30	118.36
2	A	202	CPS	O4-C4-C5	2.13	114.62	111.02
2	D	202	CPS	C8-C9-C5	2.13	107.69	103.30
2	C	203	CPS	C19-C18-C6	2.11	112.70	109.75
2	B	203	CPS	C1-C12-C13	2.11	113.28	110.48
2	A	202	CPS	C5-C6-C18	2.11	117.39	114.72
2	A	203	CPS	C11-C2-C15	-2.11	106.91	110.44
2	B	203	CPS	C11-C2-C1	-2.11	104.95	108.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	203	CPS	C15-C14-C13	2.11	115.89	112.71
2	A	201	CPS	C2-C19-C18	2.09	114.17	111.84
2	A	201	CPS	C5-C6-C18	2.09	117.37	114.72
2	B	203	CPS	O2S-S-C32	2.09	110.09	106.00
2	D	203	CPS	O3S-S-C32	2.09	109.89	106.73
2	C	201	CPS	C11-C2-C19	-2.09	108.37	111.18
2	A	201	CPS	C8-C9-C5	2.09	105.56	103.54
2	D	203	CPS	C14-C13-C12	2.08	113.15	110.62
2	C	201	CPS	C9-C5-C4	-2.07	115.80	117.67
2	D	203	CPS	C16-C15-C2	2.07	114.86	112.66
2	B	202	CPS	C1-C12-C13	2.06	113.21	110.48
2	D	201	CPS	C3-C19-C2	2.06	115.79	113.70
2	D	202	CPS	C19-C2-C15	2.05	111.36	108.51
2	D	202	CPS	O4-C4-C5	2.04	114.47	111.02
2	A	203	CPS	C5-C6-C18	2.04	117.31	114.72
2	B	203	CPS	C8-C9-C20	2.04	115.27	112.18
2	B	201	CPS	C11-C2-C1	-2.04	105.06	108.31
2	B	201	CPS	C3-C19-C2	2.04	115.77	113.70
2	A	203	CPS	C1-C12-C13	2.03	113.17	110.48
2	D	203	CPS	C1-C12-C13	2.02	113.16	110.48
2	B	202	CPS	C12-C1-C2	2.02	116.15	112.74
2	C	202	CPS	O4-C4-C5	2.02	114.43	111.02
2	D	201	CPS	C19-C18-C6	2.02	112.56	109.75
2	B	201	CPS	C9-C5-C6	-2.02	98.09	100.11
2	C	201	CPS	O4-C4-C5	2.00	114.40	111.02

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	CPS	C22-C23-C24-O1
2	A	202	CPS	C23-C24-N1-C25
2	A	203	CPS	C9-C20-C22-C23
2	B	203	CPS	C21-C20-C9-C5
2	B	203	CPS	C22-C20-C9-C5
2	B	203	CPS	C21-C20-C9-C8
2	B	203	CPS	C23-C24-N1-C25
2	C	202	CPS	C23-C24-N1-C25
2	C	202	CPS	O1-C24-N1-C25
2	C	202	CPS	N2-C30-C31-C32
2	D	201	CPS	C21-C20-C9-C5
2	D	201	CPS	C22-C20-C9-C5

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Mol	Chain	Res	Type	Atoms
2	D	201	CPS	C23-C24-N1-C25
2	D	201	CPS	O1-C24-N1-C25
2	D	201	CPS	C30-C31-C32-S
2	D	203	CPS	N2-C30-C31-C32
2	B	203	CPS	O1-C24-N1-C25
2	C	201	CPS	C21-C20-C9-C8
2	D	201	CPS	C21-C20-C9-C8
2	C	201	CPS	C21-C20-C9-C5
2	B	203	CPS	C22-C20-C9-C8
2	C	201	CPS	C22-C20-C9-C8
2	D	203	CPS	O1-C24-N1-C25
2	C	201	CPS	C22-C20-C9-C5
2	D	203	CPS	C23-C24-N1-C25
2	C	202	CPS	C31-C30-N2-C28
2	D	201	CPS	C26-C27-N2-C29
2	D	203	CPS	C26-C27-N2-C29
2	C	203	CPS	C21-C20-C22-C23
2	A	203	CPS	C21-C20-C9-C5
2	A	201	CPS	C21-C20-C22-C23
2	A	203	CPS	C21-C20-C22-C23
2	B	203	CPS	C9-C20-C22-C23
2	D	201	CPS	C9-C20-C22-C23
2	C	202	CPS	C31-C30-N2-C29
2	D	201	CPS	C26-C27-N2-C28
2	D	203	CPS	C26-C27-N2-C28
2	C	202	CPS	C31-C30-N2-C27
2	A	201	CPS	C9-C20-C22-C23
2	C	202	CPS	C9-C20-C22-C23
2	D	203	CPS	C9-C20-C22-C23
2	C	203	CPS	C9-C20-C22-C23
2	D	201	CPS	C22-C20-C9-C8
2	D	203	CPS	N1-C25-C26-C27
2	C	202	CPS	N1-C25-C26-C27
2	C	202	CPS	C21-C20-C22-C23
2	D	203	CPS	C31-C32-S-O2S
2	D	201	CPS	C26-C27-N2-C30
2	D	203	CPS	C26-C27-N2-C30
2	A	202	CPS	O1-C24-N1-C25
2	D	201	CPS	N1-C25-C26-C27
2	D	203	CPS	C22-C23-C24-N1
2	D	203	CPS	C22-C23-C24-O1
2	C	202	CPS	C26-C27-N2-C28

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Mol	Chain	Res	Type	Atoms
2	C	202	CPS	C26-C27-N2-C29
2	B	203	CPS	C25-C26-C27-N2
2	C	202	CPS	C25-C26-C27-N2
2	D	201	CPS	C25-C26-C27-N2
2	D	203	CPS	C25-C26-C27-N2
2	D	203	CPS	C22-C20-C9-C8
2	C	202	CPS	C26-C27-N2-C30
2	A	201	CPS	C20-C22-C23-C24
2	D	203	CPS	C31-C32-S-O3S
2	D	203	CPS	C31-C32-S-O1S
2	A	203	CPS	C22-C20-C9-C5
2	B	203	CPS	N1-C25-C26-C27
2	D	201	CPS	C31-C30-N2-C27
2	D	201	CPS	C21-C20-C22-C23
2	B	201	CPS	C21-C20-C9-C5
2	D	203	CPS	C22-C20-C9-C5
2	D	201	CPS	C31-C32-S-O3S
2	D	201	CPS	C31-C30-N2-C29
2	C	202	CPS	C30-C31-C32-S
2	D	203	CPS	C21-C20-C9-C8
2	A	201	CPS	C22-C20-C9-C8
2	D	203	CPS	C26-C25-N1-C24

There are no ring outliers.

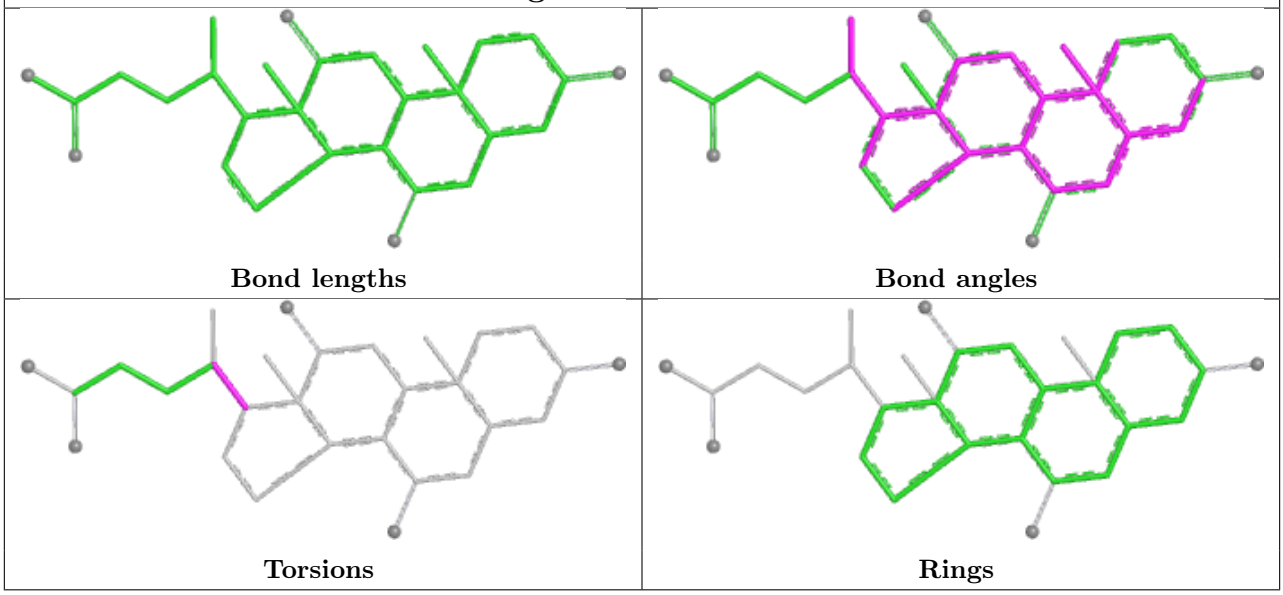
9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	203	CPS	2	0
2	C	202	CPS	2	0
2	D	202	CPS	1	0
2	D	201	CPS	2	0
2	A	201	CPS	4	0
2	C	203	CPS	2	0
2	C	201	CPS	3	0
2	A	203	CPS	2	0
2	D	203	CPS	3	0

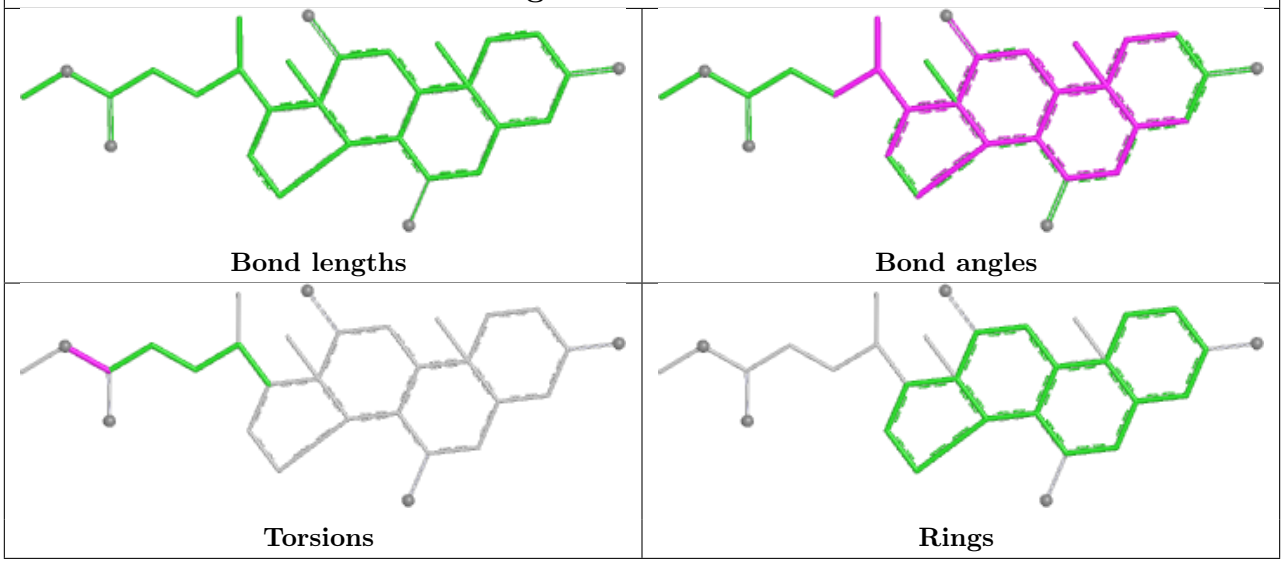
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CPS B 201



Ligand CPS A 202



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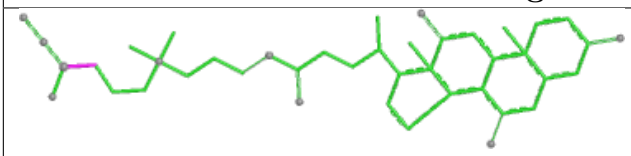

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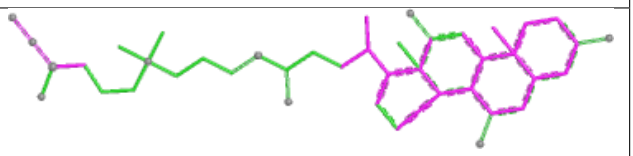
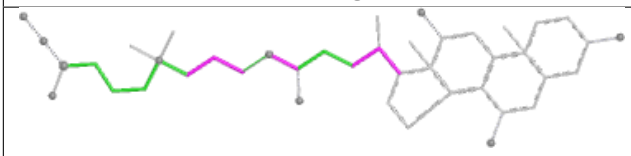
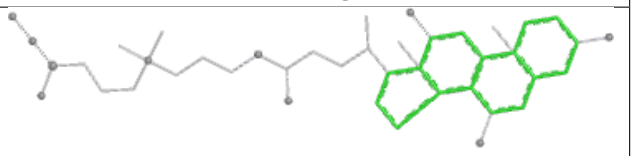


Bond angles

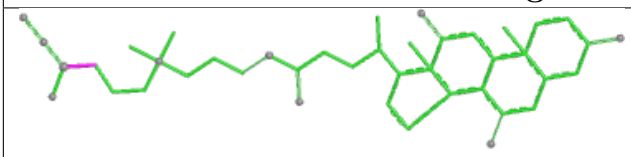


Torsions



Rings

Ligand CPS C 202



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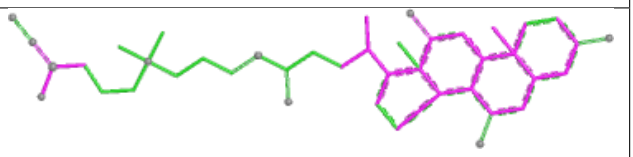
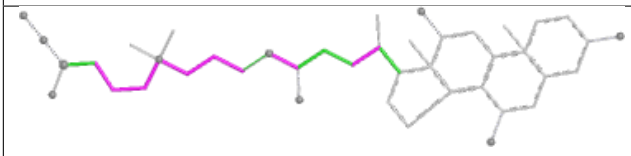


Bond angles



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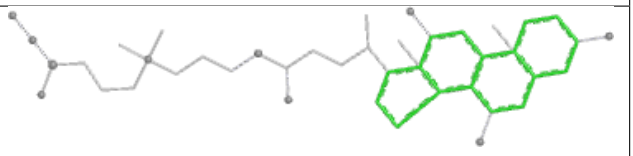

Rings

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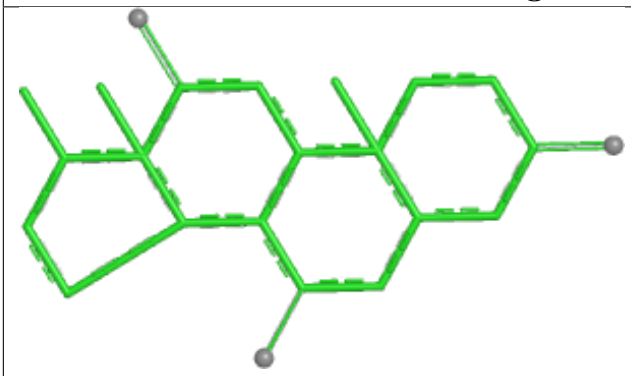
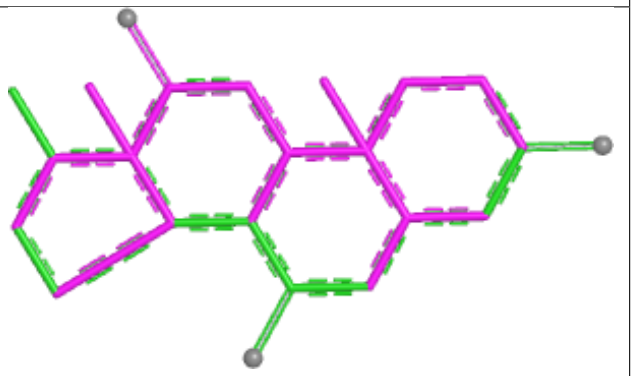
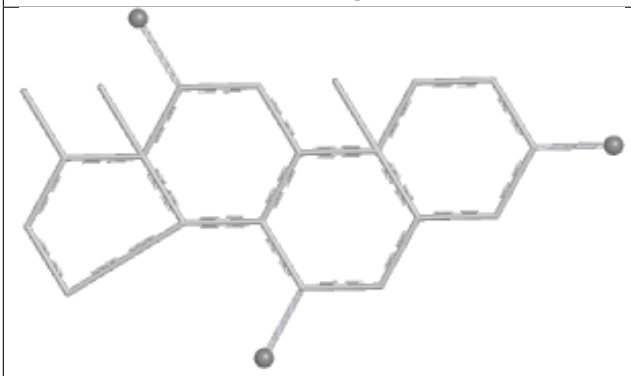


Bond lengths



Bond angles



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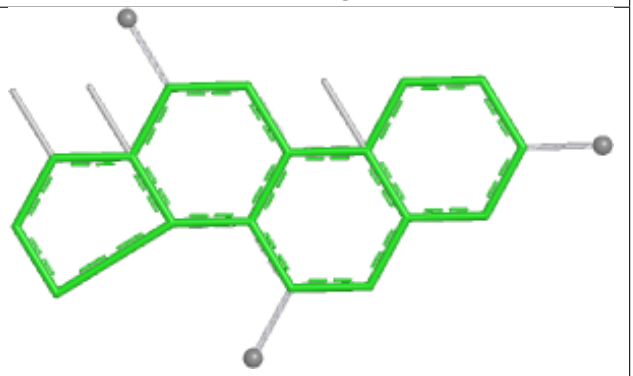

Rings

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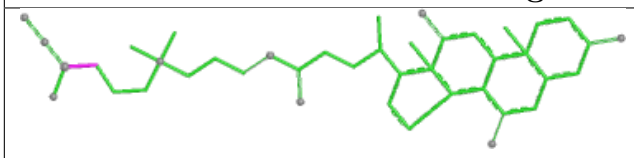

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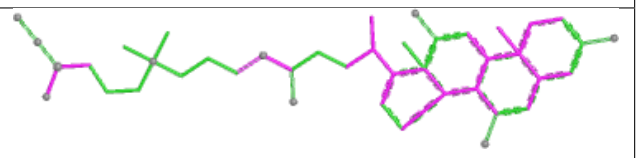
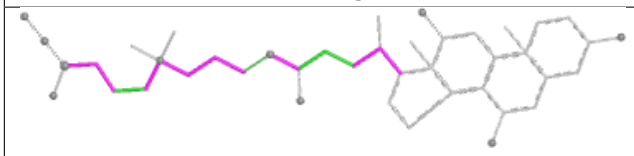


Bond angles



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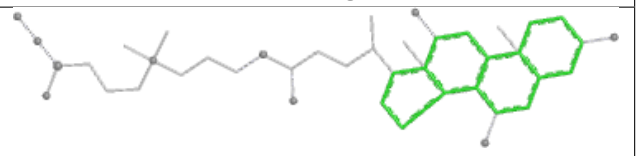

Rings

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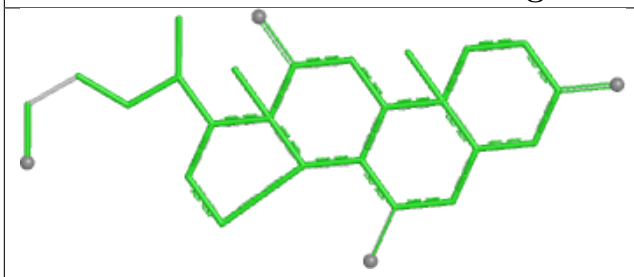

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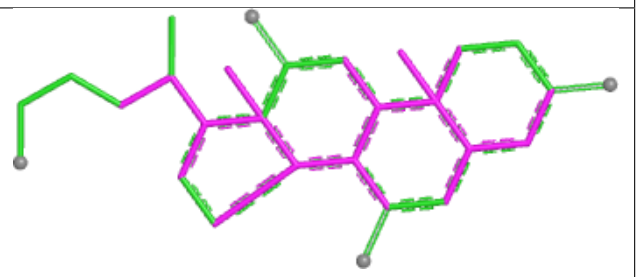

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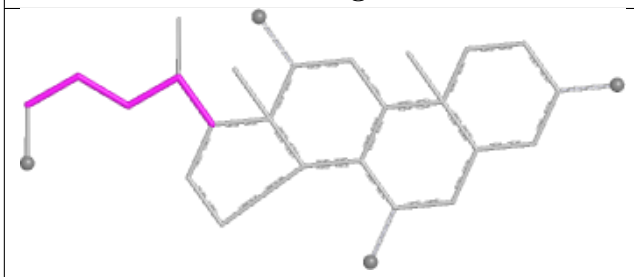

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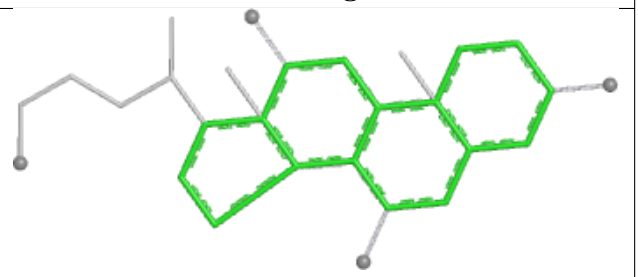
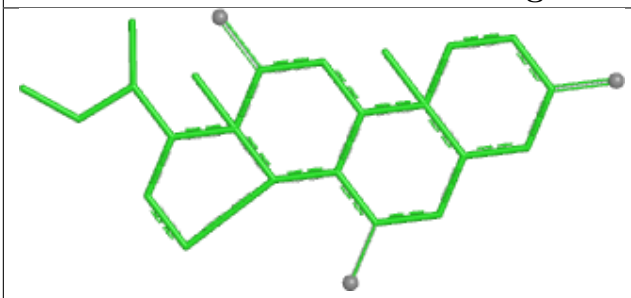


Rings

Ligand CPS C 203



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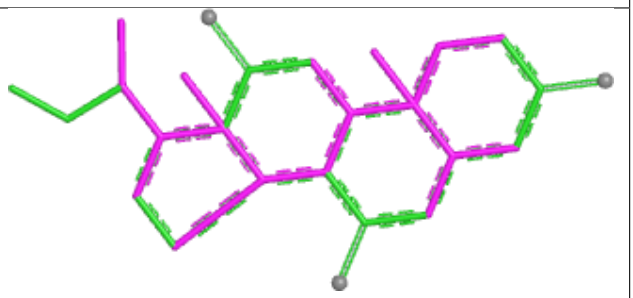

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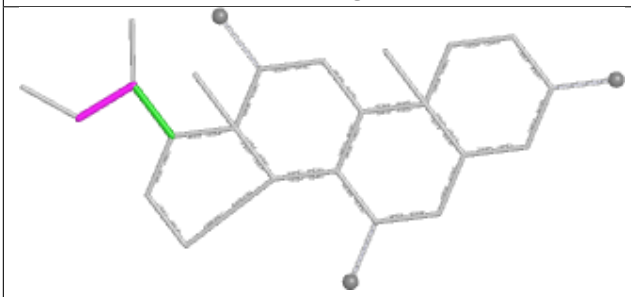

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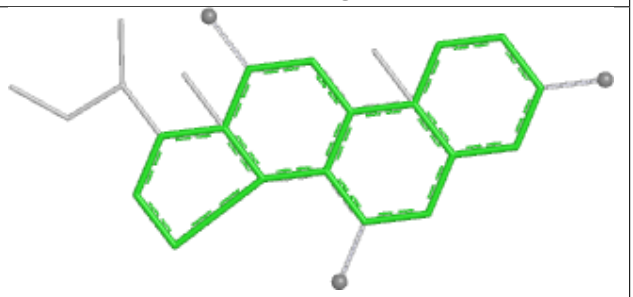

Rings

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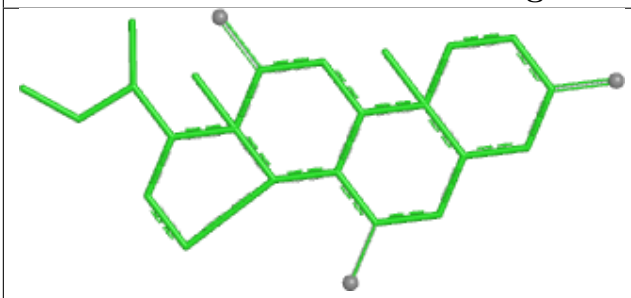

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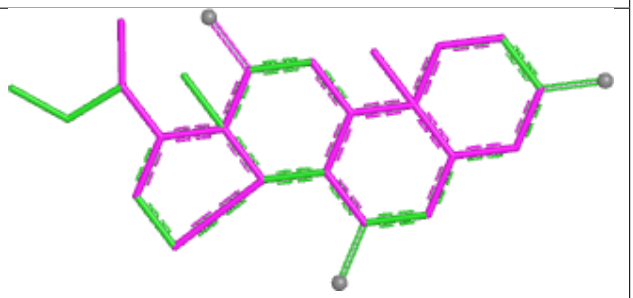

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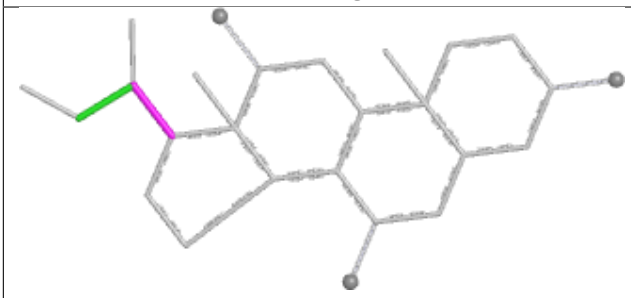

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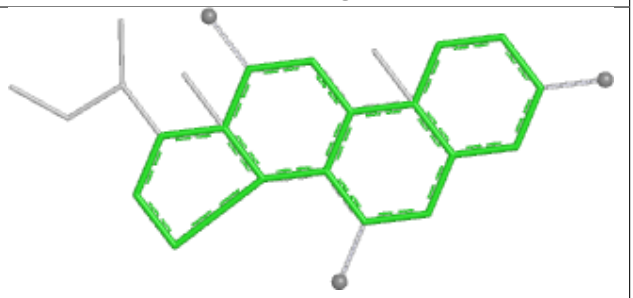
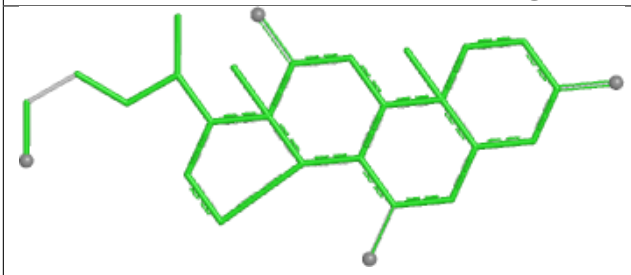


Rings

Ligand CPS A 203



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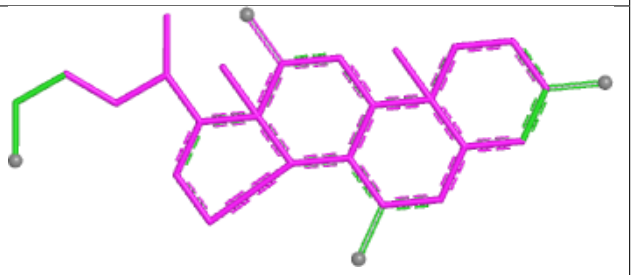
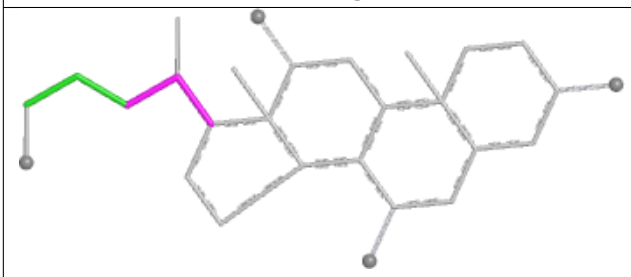
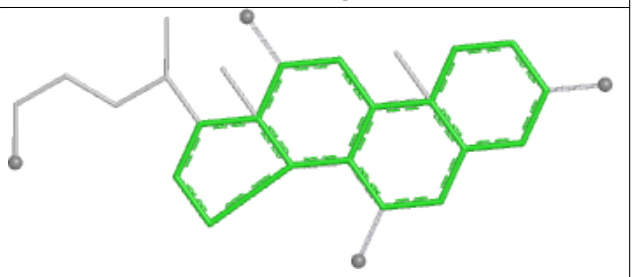


Bond angles

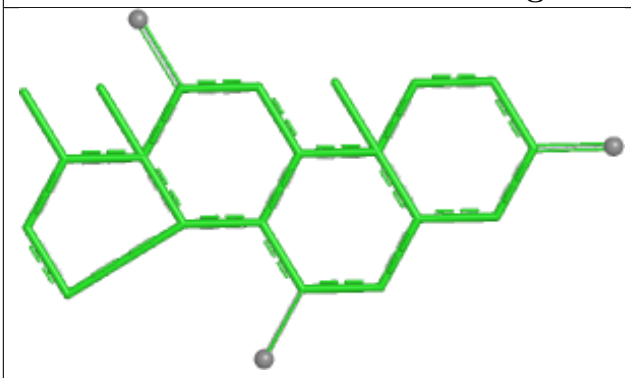


Torsions

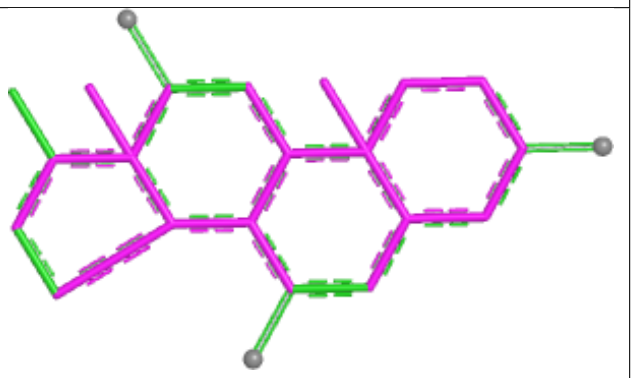


Rings

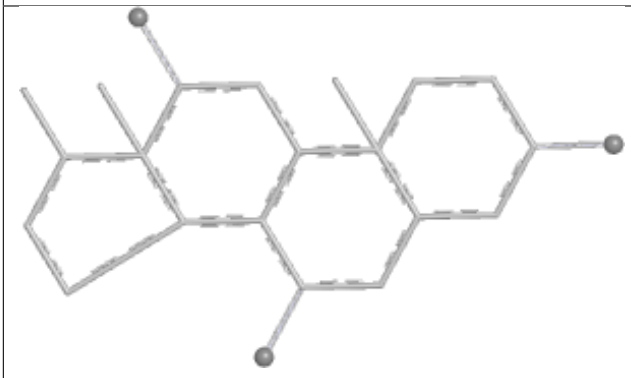
Ligand CPS B 202



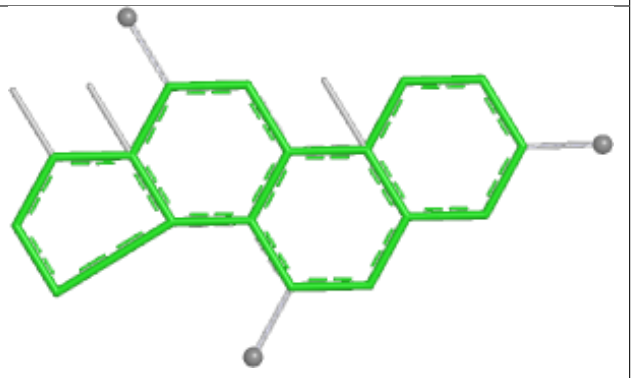
Bond lengths



Bond angles

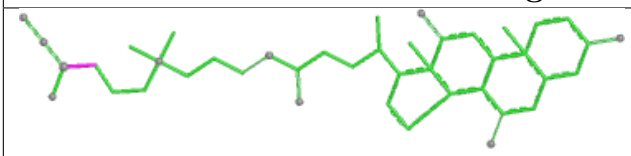


Torsions

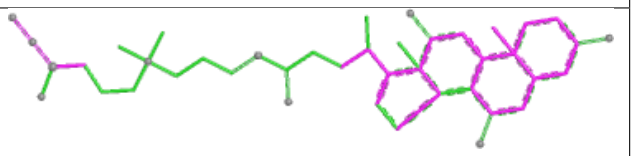


Rings

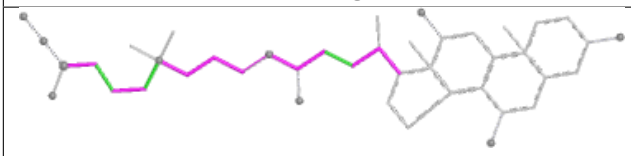
Ligand CPS D 203



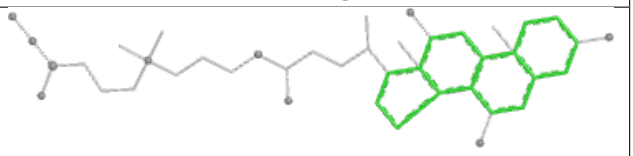
Bond lengths



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	157/157 (100%)	0.57	13 (8%)	17	20	22, 41, 74, 87	0
1	B	156/157 (99%)	0.47	10 (6%)	25	30	19, 40, 72, 98	0
1	C	157/157 (100%)	0.36	7 (4%)	38	44	21, 39, 68, 89	0
1	D	157/157 (100%)	0.70	16 (10%)	12	14	18, 47, 80, 97	1 (0%)
All	All	627/628 (99%)	0.53	46 (7%)	21	25	18, 42, 76, 98	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	CYS	4.3
1	A	157	ASP	4.1
1	D	133	LEU	4.0
1	D	68	CYS	3.5
1	A	42	ALA	3.2
1	B	38	CYS	3.1
1	A	108	GLY	3.1
1	D	40	ASP	3.0
1	D	132	ASP	3.0
1	D	157	ASP	2.9
1	D	34	THR	2.7
1	D	38	CYS	2.7
1	A	38	CYS	2.7
1	C	131	ARG	2.7
1	B	110	ASP	2.6
1	B	69	GLU	2.6
1	B	68	CYS	2.5
1	C	157	ASP	2.5
1	C	16	ASN	2.5
1	D	42	ALA	2.5
1	B	132	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	35	ASP	2.5
1	D	15	LEU	2.4
1	B	156	GLU	2.4
1	D	36	SER	2.4
1	D	84	LYS	2.4
1	A	133	LEU	2.3
1	A	105	SER	2.3
1	A	110	ASP	2.3
1	A	41	ASN	2.2
1	B	112	LYS	2.2
1	D	30	PHE	2.2
1	A	132	ASP	2.1
1	B	155	ASN	2.1
1	B	34	THR	2.1
1	C	142	ASP	2.1
1	C	109	HIS	2.1
1	D	154	GLN	2.1
1	D	106	VAL	2.1
1	A	69	GLU	2.1
1	A	143	GLU	2.1
1	C	36	SER	2.0
1	D	69	GLU	2.0
1	B	109	HIS	2.0
1	C	38	CYS	2.0
1	A	144	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

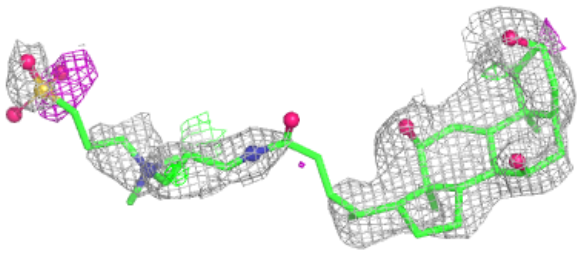
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

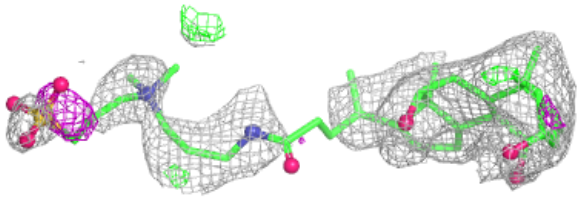
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	204	5/5	0.46	0.20	124,124,124,125	0
2	CPS	B	203	42/42	0.67	0.18	54,69,115,116	0
3	SO4	B	204	5/5	0.69	0.18	135,135,135,135	0
3	SO4	A	205	5/5	0.74	0.15	111,112,112,112	0
3	SO4	A	204	5/5	0.76	0.17	108,109,109,109	0
2	CPS	D	201	42/42	0.76	0.16	53,62,114,116	0
2	CPS	D	203	42/42	0.77	0.17	58,67,103,105	0
2	CPS	D	202	23/42	0.78	0.22	81,83,84,85	0
2	CPS	C	202	42/42	0.79	0.17	57,70,110,111	0
2	CPS	A	203	28/42	0.80	0.17	71,79,81,81	0
2	CPS	C	201	26/42	0.81	0.26	90,92,93,94	0
2	CPS	A	202	30/42	0.83	0.15	58,63,68,71	0
2	CPS	C	203	26/42	0.84	0.16	63,65,67,68	0
2	CPS	B	201	29/42	0.84	0.17	65,67,72,75	0
2	CPS	A	201	28/42	0.85	0.12	42,49,58,61	0
2	CPS	B	202	23/42	0.86	0.12	55,59,64,66	0

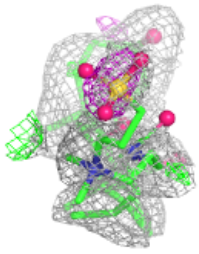
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CPS B 203:

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

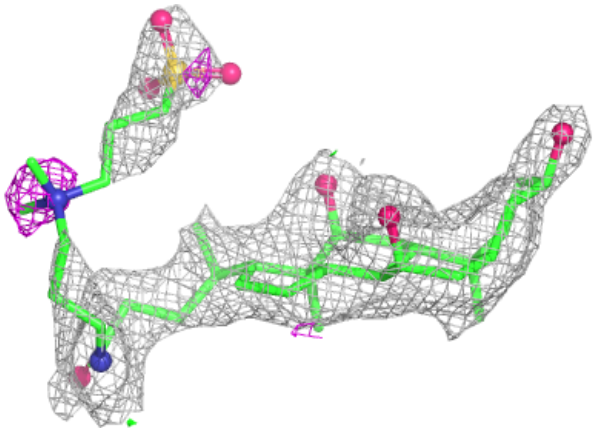


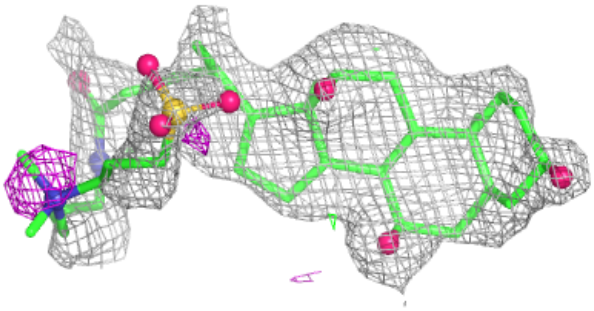


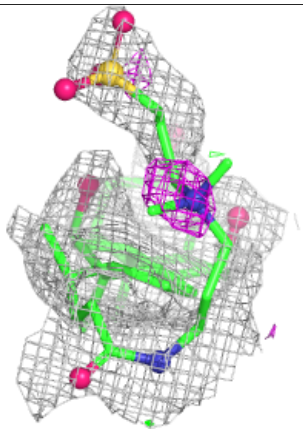


Electron density around CPS D 201:

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

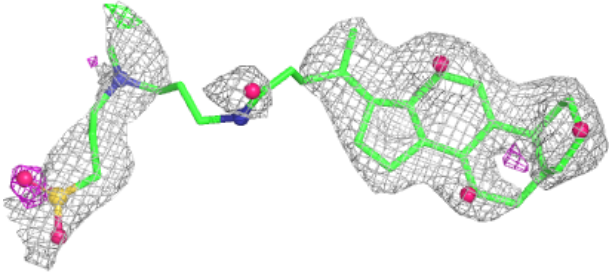


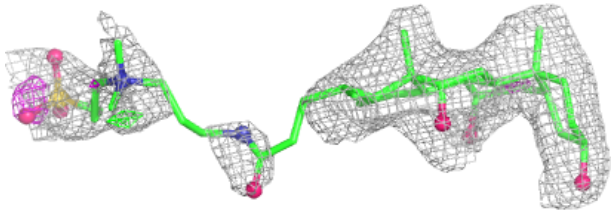


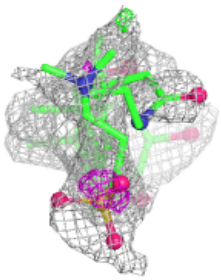


Electron density around CPS D 203:

$2mF_o$-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 D 202:

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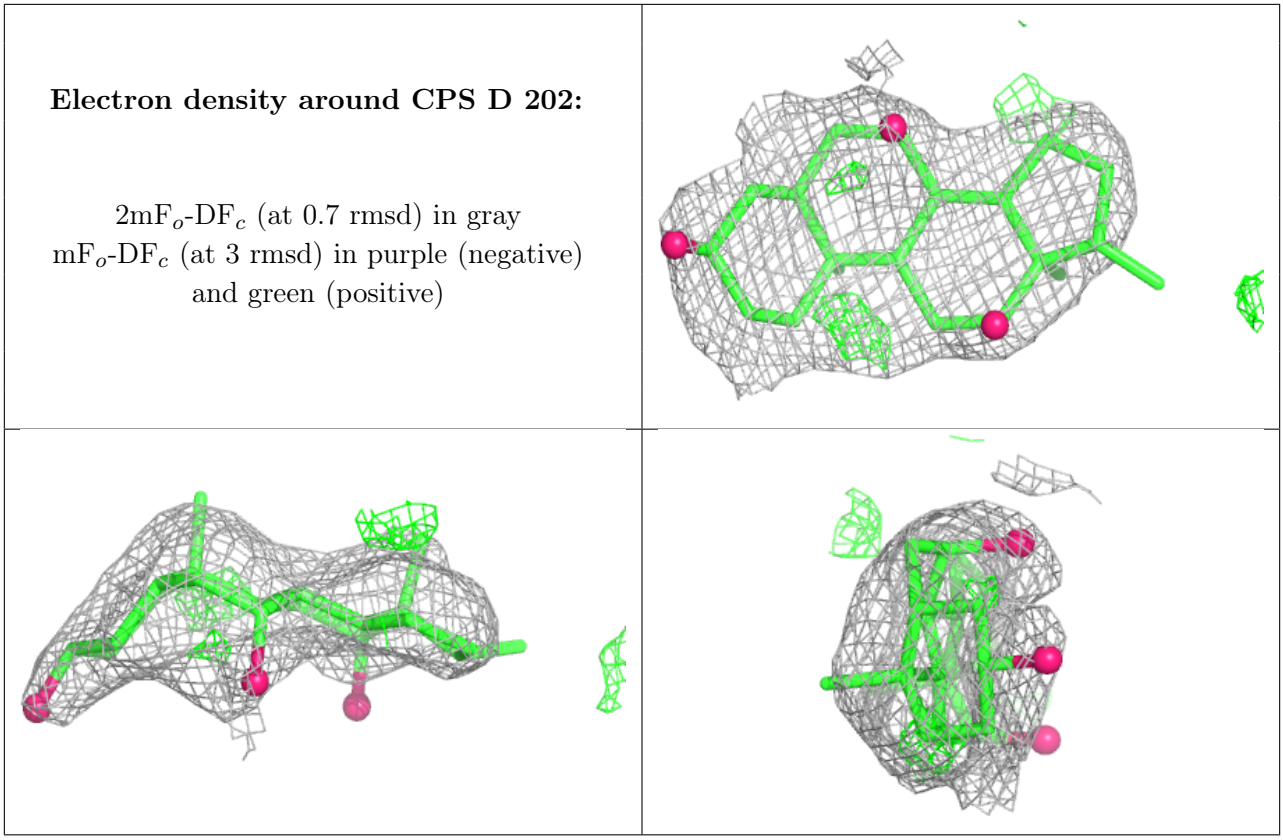
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CPS C 202:

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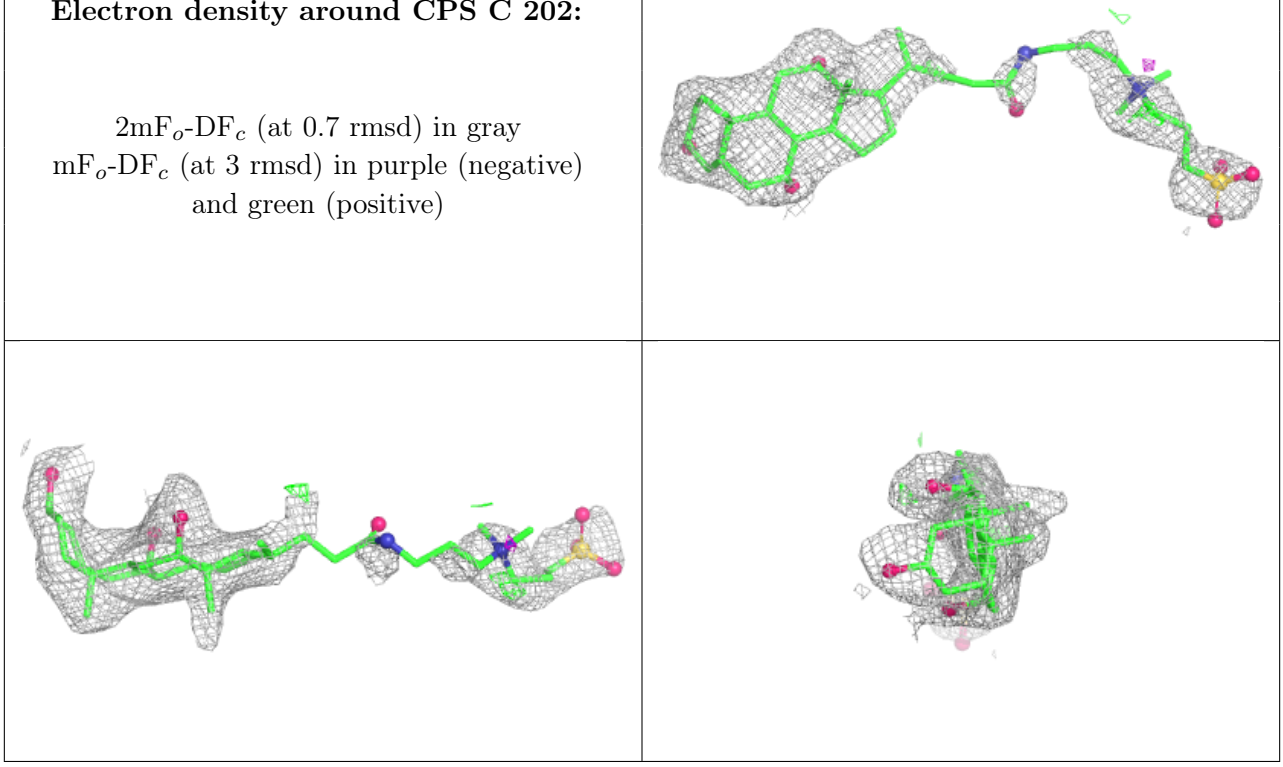
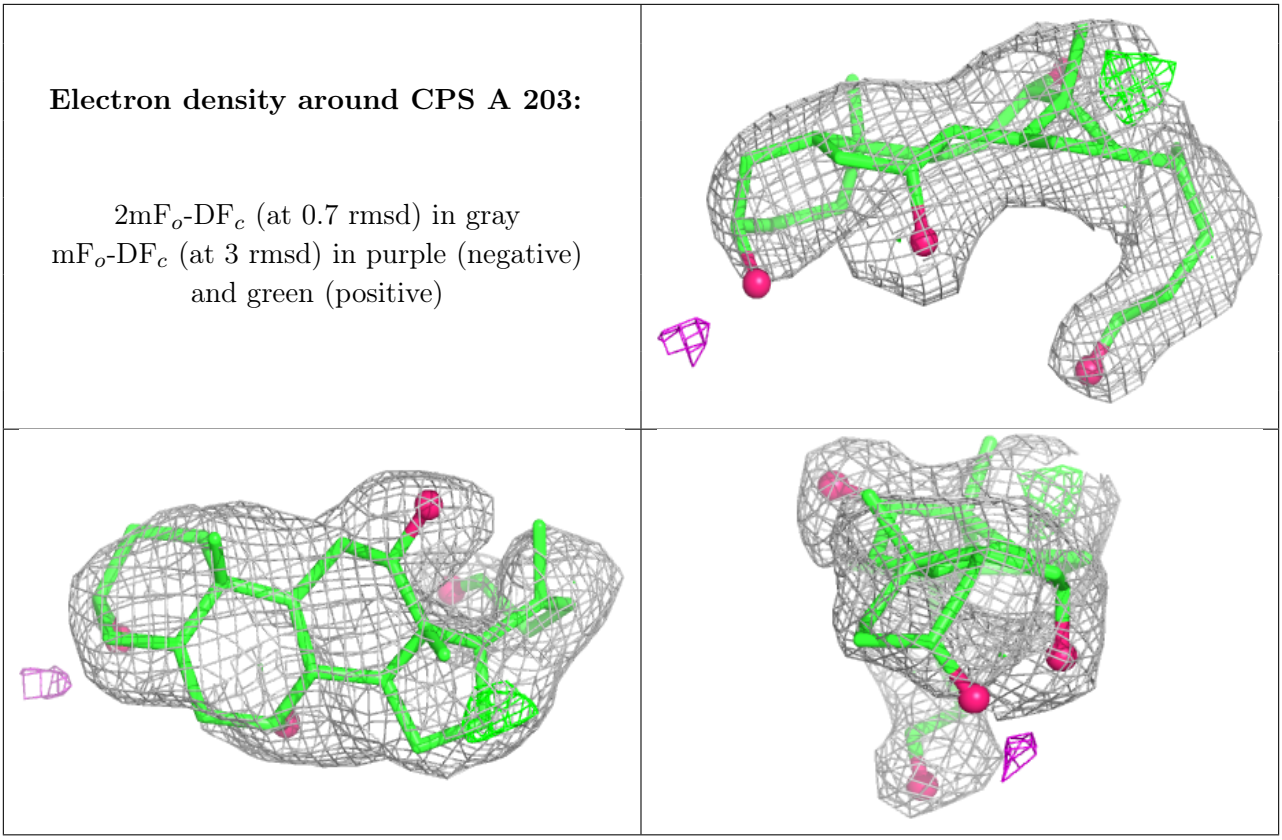
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



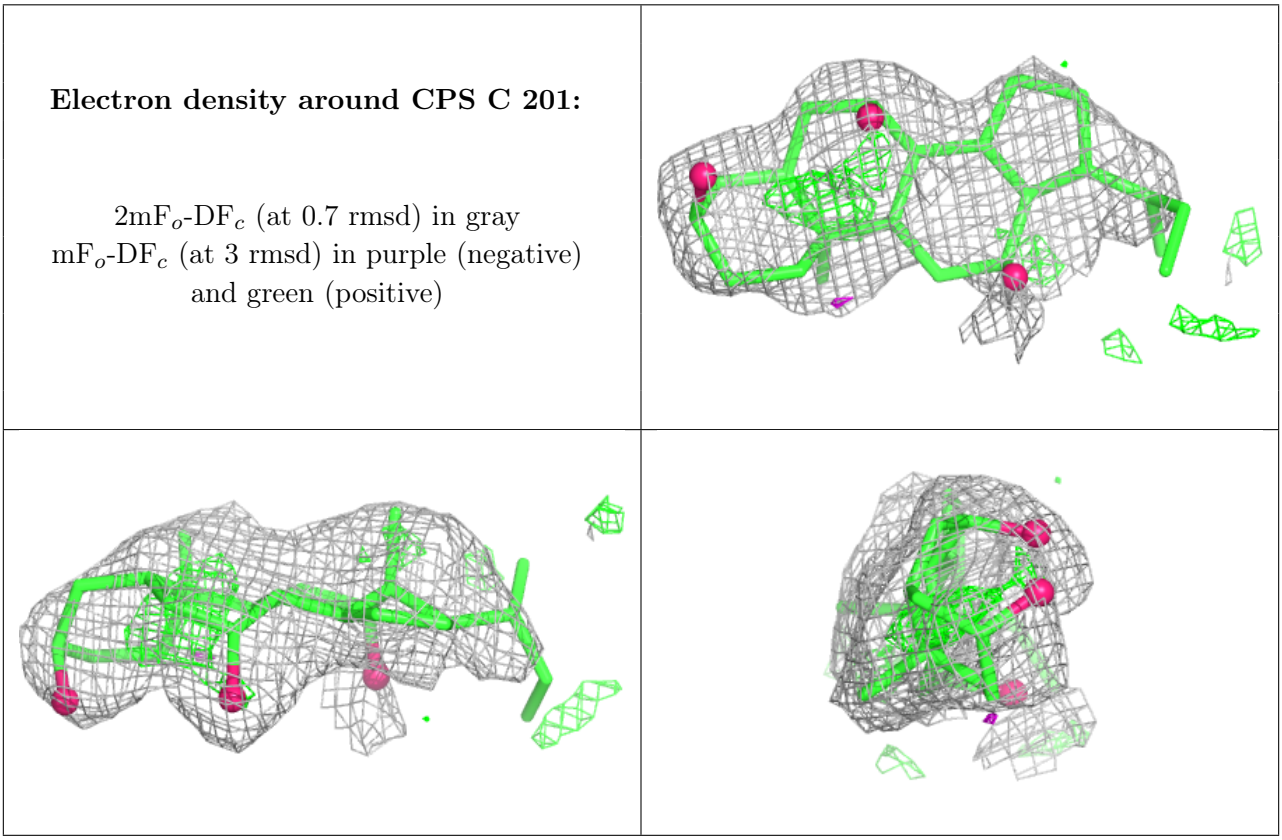
Electron density around CPS A 203:

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



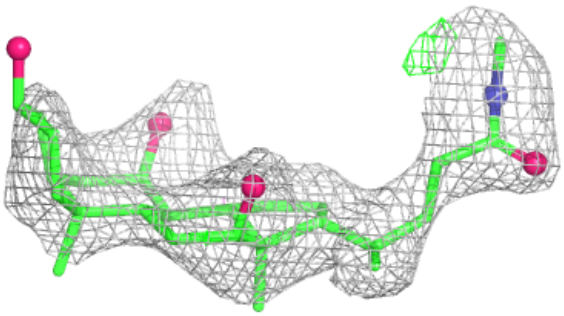
Electron density around CPS C 201:

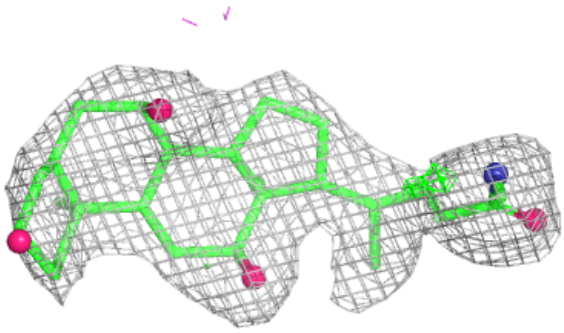
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

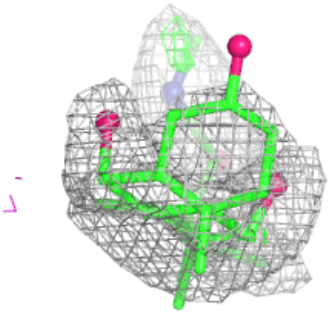


Electron density around CPS A 202:

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

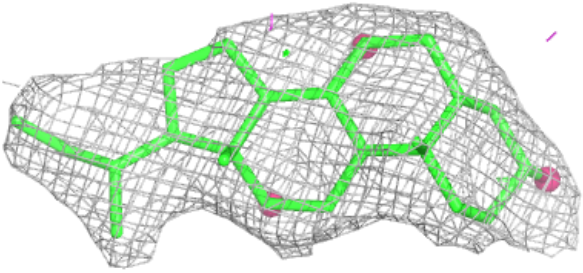


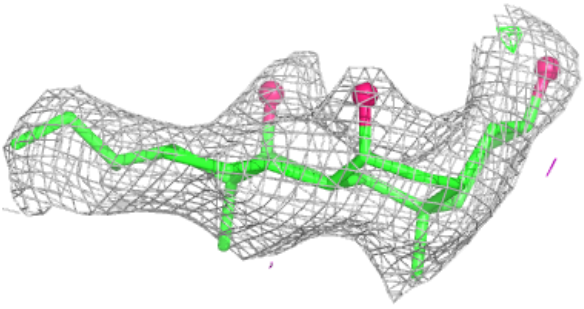


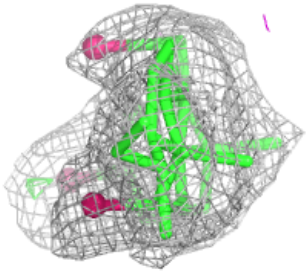


Electron density around CPS C 203:

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

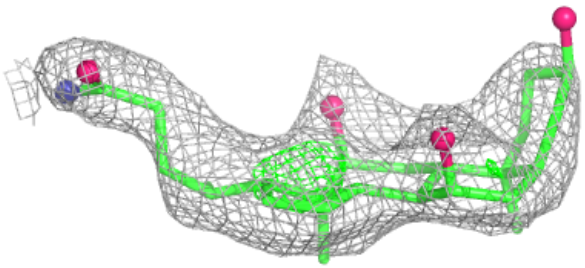


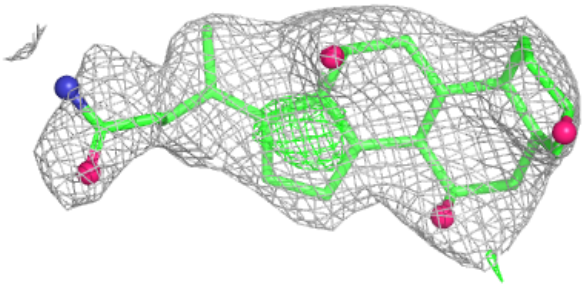


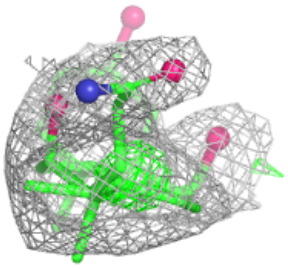


Electron density around CPS B 201:

$2mF_o$-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 201:

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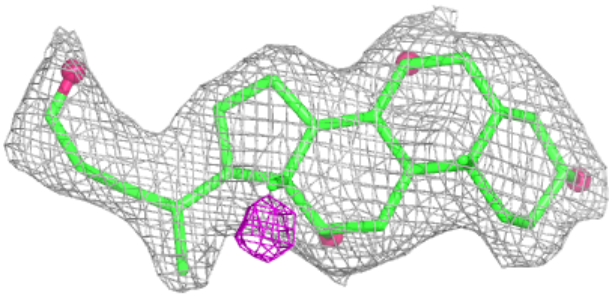
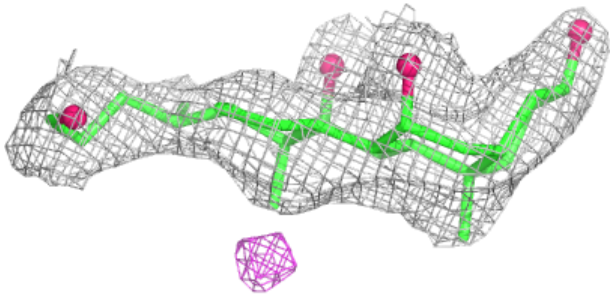
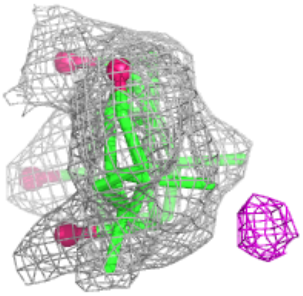
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around CPS B 202:

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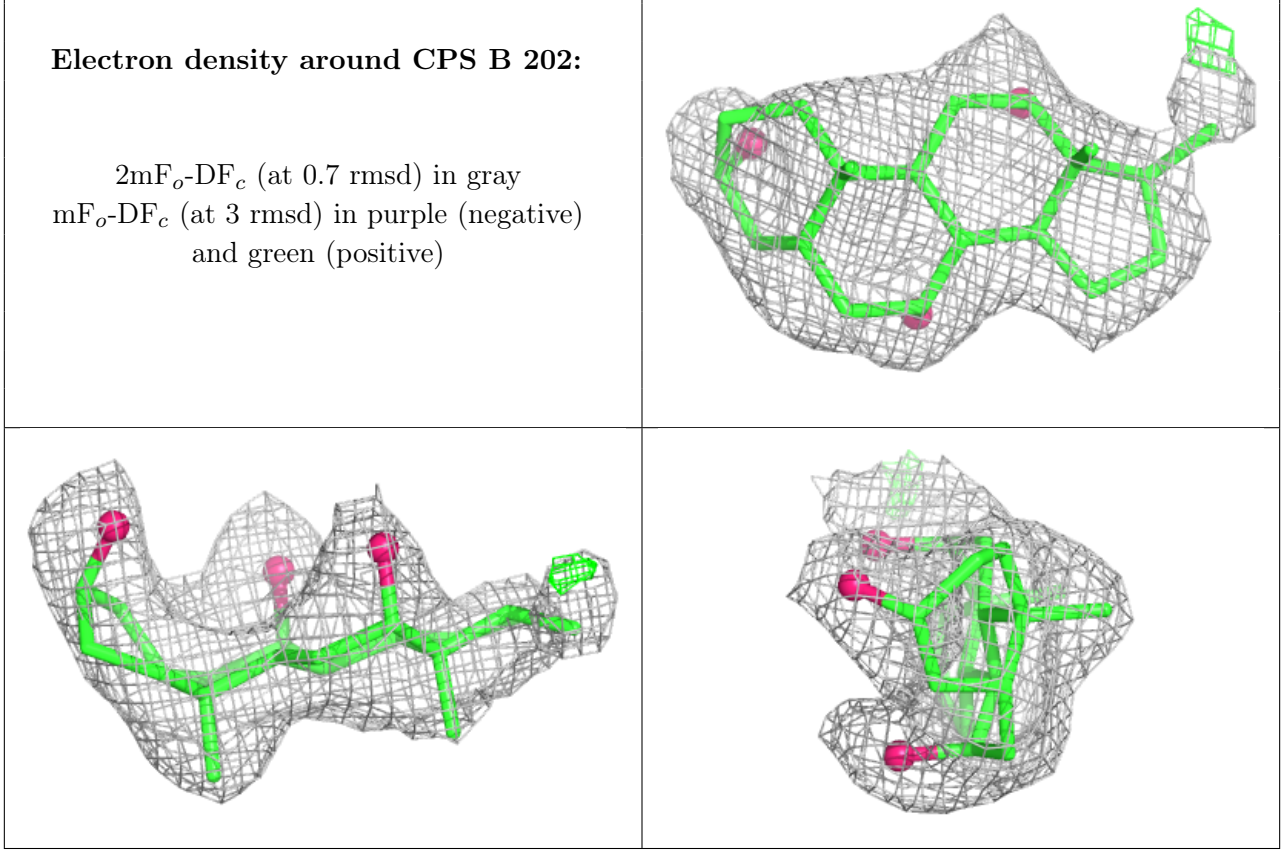
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.