Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 01:09 AM UTC

PDB ID	:	5WB2 / pdb_00005wb2
Title	:	US28 bound to engineered chemokine CX3CL1.35 and nanobodies
Authors	:	Jude, K.M.; Burg, J.S.; Tsutsumi, N.; Miles, T.F.; Garcia, K.C.
Deposited on	:	2017-06-27
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

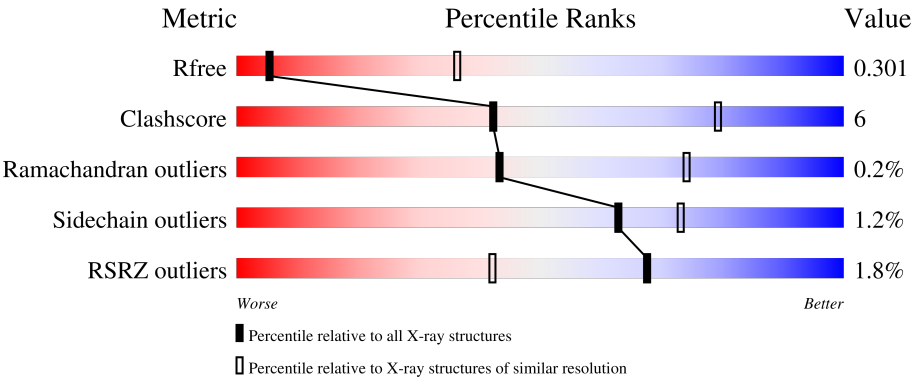
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	460	2% 77% 15% 8%
2	B	76	3% 82% 12%
3	D	131	% 82% 14%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4907 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 Envelope protein US28, nanobody 7 fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3287	2160	520	583	24			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	TYR	-	expression tag	UNP Q80KM9
A	-5	LYS	-	expression tag	UNP Q80KM9
A	-4	ASP	-	expression tag	UNP Q80KM9
A	-3	ASP	-	expression tag	UNP Q80KM9
A	-2	ASP	-	expression tag	UNP Q80KM9
A	-1	ASP	-	expression tag	UNP Q80KM9
A	0	ALA	-	expression tag	UNP Q80KM9

- Molecule 2 is a protein called CX3CL1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	0
			531	336	95	94	6			

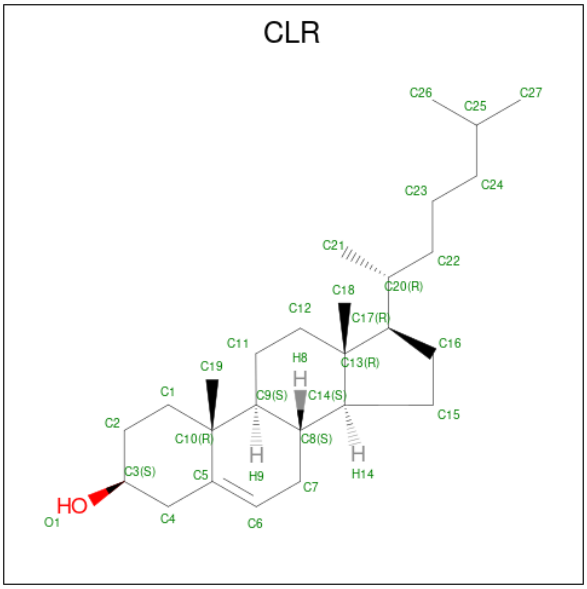
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	LEU	-	expression tag	UNP Q6I9S9
B	2	LEU	-	expression tag	UNP Q6I9S9
B	3	PRO	-	expression tag	UNP Q6I9S9
B	4	HIS	-	expression tag	UNP Q6I9S9
B	5	ALA	-	expression tag	UNP Q6I9S9
B	6	ASN	-	expression tag	UNP Q6I9S9
B	7	TYR	-	expression tag	UNP Q6I9S9
B	8	CYS	-	expression tag	UNP Q6I9S9
B	9	ALA	-	expression tag	UNP Q6I9S9

- Molecule 3 is a protein called nanobody B1.

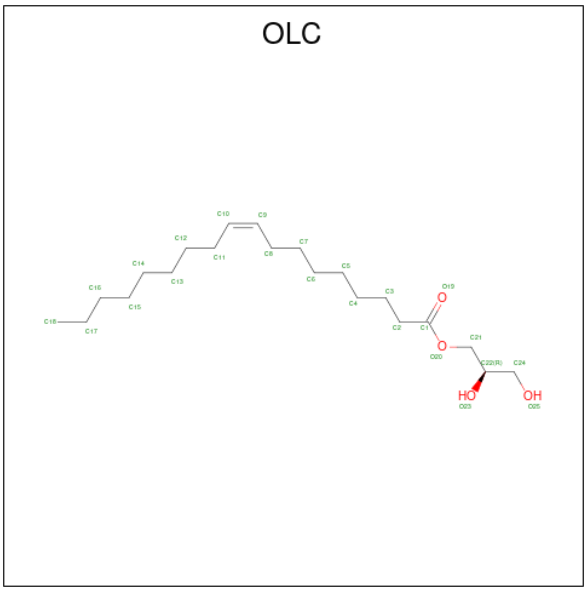
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	127	Total	C	N	O	S	0	0	0
			937	585	155	192	5			

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			28	27	1			
4	A	1	Total	C	O		0	0
			28	27	1			

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).

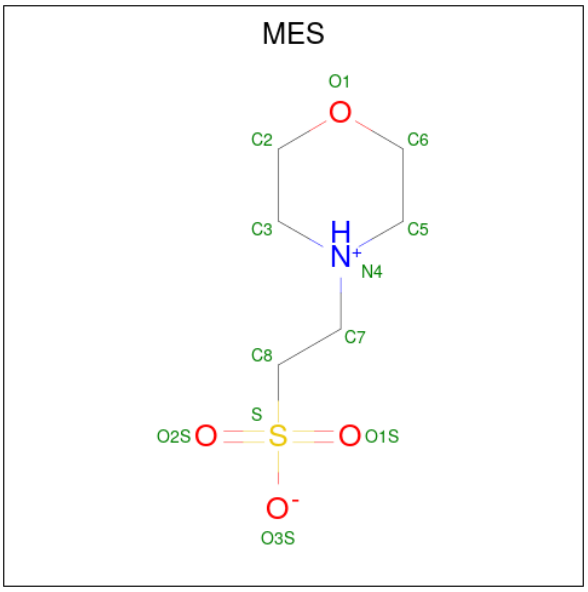


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 25 21 4	0	0
5	A	1	Total C O 25 21 4	0	0
5	A	1	Total C O 25 21 4	0	0
5	A	1	Total C 8 8	0	0

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).

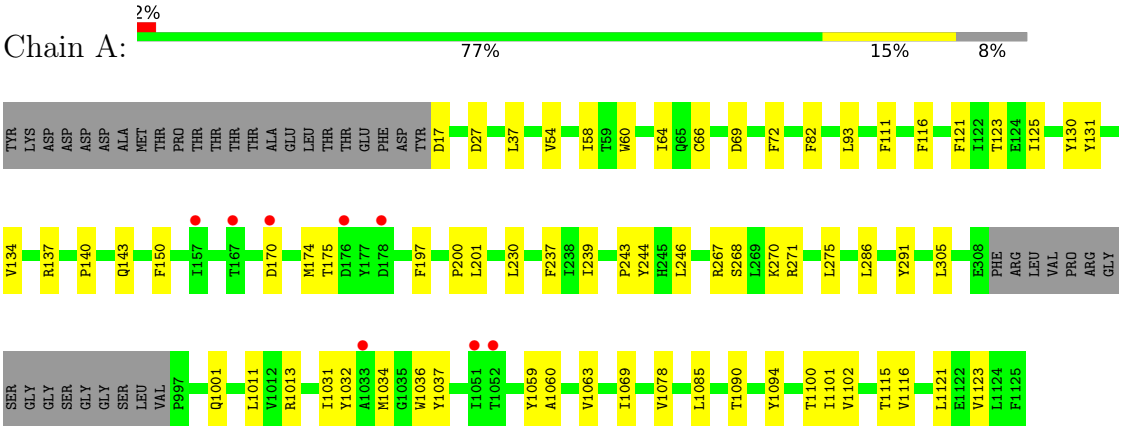


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	B	1	12	6	1	4	1	0	0

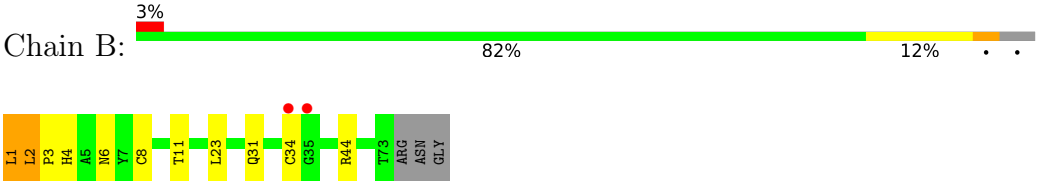
3 Residue-property plots (i)

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.

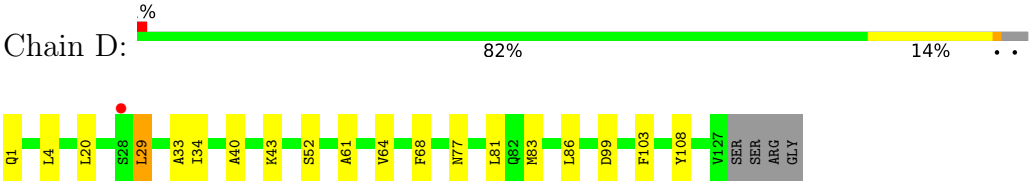
• Molecule 1: Envelope protein US28, nanobody 7 fusion protein



• Molecule 2: CX3CL1 protein



• Molecule 3: nanobody B1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	47.17Å 128.94Å 127.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.37 – 3.50 45.37 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.37-3.50) 89.5 (45.37-3.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.252 , 0.296 0.257 , 0.301	Depositor DCC
R_{free} test set	1041 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å^2)	80.9	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.033 for -h,l,k	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4907	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: MES, CLR, ZN, PCA, YCM, OLC

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	0.13	0/3348	0.45	0/4569
2	B	0.09	0/542	0.27	0/740
3	D	0.12	0/949	0.32	0/1290
All	All	0.13	0/4839	0.41	0/6599

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3287	0	3231	42	0
2	B	531	0	495	10	0
3	D	937	0	849	11	0
4	A	56	0	92	8	0
5	A	83	0	135	4	0
6	B	1	0	0	0	0
7	B	12	0	12	5	0
All	All	4907	0	4814	61	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 6.

All (61) 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:270:LYS:NZ	2:B:8:CYS:SG	2.50	0.84
1:A:271:ARG:HD2	4:A:1202:CLR:H12	1.62	0.82
1:A:174:MET:HE1	2:B:34:CYS:HA	1.72	0.72
2:B:3:PRO:HA	7:B:102:MES:H82	1.72	0.70
2:B:6:ASN:ND2	7:B:102:MES:O3S	2.26	0.69
1:A:64:ILE:HG23	1:A:69:ASP:HB2	1.76	0.67
1:A:246:LEU:HD23	4:A:1201:CLR:H151	1.77	0.65
1:A:1011:LEU:HD21	1:A:1013:ARG:HH12	1.63	0.64
1:A:243:PRO:HG3	4:A:1201:CLR:H222	1.84	0.59
1:A:239:ILE:HG22	4:A:1201:CLR:H263	1.84	0.57
3:D:83:MET:HB3	3:D:86:LEU:HD21	1.85	0.57
3:D:52:SER:HB2	3:D:108:TYR:O	2.03	0.57
1:A:175:THR:OG1	7:B:102:MES:O1S	2.19	0.56
1:A:1090:THR:HG23	1:A:1115:THR:HA	1.89	0.54
3:D:20:LEU:HD12	3:D:81:LEU:HD23	1.90	0.54
2:B:11:THR:HG22	2:B:34:CYS:HB2	1.89	0.53
3:D:33:ALA:O	3:D:99:ASP:N	2.32	0.53
1:A:1100:THR:O	1:A:1102:VAL:N	2.41	0.52
1:A:131:TYR:HB3	1:A:137:ARG:HB3	1.93	0.51
1:A:1037:TYR:O	1:A:1094:TYR:N	2.34	0.51
1:A:17:ASP:N	1:A:17:ASP:OD1	2.44	0.51
1:A:123:THR:HG21	5:A:1206:OLC:H12A	1.94	0.49
1:A:244:TYR:CE2	2:B:2:LEU:HD22	2.47	0.49
3:D:103:PHE:HB2	3:D:108:TYR:CD1	2.47	0.49
1:A:54:VAL:O	1:A:58:ILE:HG13	2.13	0.48
1:A:230:LEU:HD21	1:A:1101:ILE:HD13	1.96	0.48
1:A:1034:MET:HB2	1:A:1078:VAL:HG21	1.94	0.48
3:D:61:ALA:HB3	3:D:64:VAL:HG12	1.97	0.47
1:A:201:LEU:HD13	1:A:237:PHE:CD2	2.50	0.46
1:A:121:PHE:O	1:A:125:ILE:HG12	2.15	0.46
1:A:1085:LEU:HB3	1:A:1116:VAL:HG21	1.96	0.46
1:A:1060:ALA:HB3	1:A:1063:VAL:HG12	1.97	0.45
3:D:29:LEU:HD12	3:D:77:ASN:HB3	1.97	0.45
1:A:1059:TYR:OH	1:A:1069:ILE:HG22	2.17	0.45
2:B:23:LEU:O	2:B:44:ARG:N	2.49	0.45
1:A:116:PHE:HD1	5:A:1206:OLC:H17	1.82	0.44
1:A:170:ASP:HB3	2:B:31:GLN:O	2.18	0.44
3:D:68:PHE:HB3	3:D:81:LEU:HD11	2.00	0.43
1:A:27:ASP:OD1	1:A:267:ARG:NH2	2.51	0.43
3:D:29:LEU:HD23	3:D:34:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:29:LEU:CD1	3:D:29:LEU:H	2.32	0.42
3:D:40:ALA:HB3	3:D:43:LYS:HD2	2.02	0.42
4:A:1202:CLR:H182	4:A:1202:CLR:H8	1.79	0.42
1:A:66:YCM:HD3	1:A:1032:TYR:CE2	2.55	0.42
1:A:140:PRO:HG2	1:A:143:GLN:HG3	2.01	0.42
2:B:1:LEU:O	7:B:102:MES:H52	2.20	0.42
1:A:275:LEU:HD13	4:A:1202:CLR:H122	2.02	0.41
1:A:82:PHE:HE1	1:A:111:PHE:CE1	2.38	0.41
1:A:268:SER:HB3	4:A:1202:CLR:H41	2.02	0.41
1:A:60:TRP:CD1	1:A:305:LEU:HD22	2.56	0.41
1:A:130:TYR:O	1:A:134:VAL:HG12	2.20	0.41
4:A:1201:CLR:H111	4:A:1201:CLR:H193	1.79	0.41
2:B:4:HIS:N	7:B:102:MES:O2S	2.45	0.41
1:A:72:PHE:CE1	1:A:291:TYR:HB3	2.55	0.41
1:A:150:PHE:HZ	5:A:1204:OLC:H5A	1.86	0.41
1:A:1031:ILE:HG21	1:A:1034:MET:HE3	2.02	0.41
1:A:197:PHE:C	1:A:200:PRO:HD2	2.45	0.41
1:A:201:LEU:HD13	1:A:237:PHE:HD2	1.85	0.41
1:A:286:LEU:HD12	5:A:1203:OLC:H8	2.03	0.41
1:A:1036:TRP:HE1	1:A:1078:VAL:HG12	1.86	0.41
1:A:37:LEU:HD21	1:A:93:LEU: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	415/460 (90%)	403 (97%)	11 (3%)	1 (0%)	43 74
2	B	71/76 (93%)	66 (93%)	5 (7%)	0	100 100
3	D	125/131 (95%)	118 (94%)	7 (6%)	0	100 100
All	All	611/667 (92%)	587 (96%)	23 (4%)	1 (0%)	43 74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1001	GLN

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	348/399 (87%)	346 (99%)	2 (1%)	78	79
2	B	50/64 (78%)	48 (96%)	2 (4%)	28	54
3	D	93/103 (90%)	91 (98%)	2 (2%)	45	65
All	All	491/566 (87%)	485 (99%)	6 (1%)	63	73

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1121	LEU
1	A	1123	VAL
2	B	1	LEU
2	B	2	LEU
3	D	4	LEU
3	D	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	303	HIS
1	A	1073	ASN
1	A	1083	ASN
2	B	4	HIS
2	B	28	GLN
2	B	31	GLN
2	B	45	GLN
3	D	124	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)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	YCM	A	304	1	7,9,10	1.14	0	5,10,12	0.55	0
1	YCM	A	66	1	7,9,10	1.15	0	5,10,12	0.48	0
3	PCA	D	1	3	7,8,9	1.91	1 (14%)	9,10,12	2.19	5 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YCM	A	304	1	-	3/6/8/10	-
1	YCM	A	66	1	-	2/6/8/10	-
3	PCA	D	1	3	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	PCA	CD-N	4.93	1.46	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	PCA	CA-N-CD	-3.02	103.22	113.58
3	D	1	PCA	OE-CD-CG	-3.01	121.35	126.72
3	D	1	PCA	CB-CA-N	2.79	110.91	103.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	PCA	CG-CD-N	2.60	114.75	108.39
3	D	1	PCA	CB-CA-C	-2.26	109.56	112.66

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	YCM	SG-CD-CE-NZ2
1	A	304	YCM	SG-CD-CE-OZ1
1	A	304	YCM	SG-CD-CE-NZ2
1	A	304	YCM	CA-CB-SG-CD
1	A	66	YCM	SG-CD-CE-OZ1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	YCM	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	OLC	A	1205	-	24,24,24	0.62	0	25,25,25	0.94	1 (4%)
5	OLC	A	1203	-	24,24,24	0.61	0	25,25,25	1.01	2 (8%)
4	CLR	A	1202	-	31,31,31	0.61	0	48,48,48	1.65	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MES	B	102	-	12,12,12	2.34	1 (8%)	15,16,16	1.96	4 (26%)
5	OLC	A	1206	-	7,7,24	0.22	0	6,6,25	0.72	0
4	CLR	A	1201	-	31,31,31	0.94	1 (3%)	48,48,48	1.35	5 (10%)
5	OLC	A	1204	-	24,24,24	0.60	0	25,25,25	0.98	2 (8%)

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
5	OLC	A	1205	-	-	5/24/24/24	-
5	OLC	A	1203	-	-	13/24/24/24	-
4	CLR	A	1202	-	-	5/10/68/68	0/4/4/4
7	MES	B	102	-	-	3/6/14/14	0/1/1/1
5	OLC	A	1206	-	-	1/5/5/24	-
4	CLR	A	1201	-	-	6/10/68/68	0/4/4/4
5	OLC	A	1204	-	-	6/24/24/24	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	102	MES	C8-S	-7.87	1.66	1.77
4	A	1201	CLR	C20-C17	2.74	1.59	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	102	MES	C5-N4-C3	5.20	120.05	108.84
4	A	1202	CLR	C13-C14-C8	-4.93	107.42	114.41
4	A	1202	CLR	C13-C17-C20	-4.61	112.37	119.50
4	A	1202	CLR	C7-C8-C9	3.87	114.19	109.72
4	A	1201	CLR	C11-C9-C10	-3.47	108.80	113.08
4	A	1201	CLR	C10-C9-C8	-3.32	107.87	112.71
4	A	1201	CLR	C13-C14-C8	-3.30	109.73	114.41
4	A	1202	CLR	C11-C9-C10	-2.64	109.83	113.08
4	A	1202	CLR	C14-C8-C9	-2.62	105.67	109.09
7	B	102	MES	C7-N4-C3	2.61	118.18	111.24
4	A	1202	CLR	C2-C3-C4	-2.39	106.93	110.29
4	A	1202	CLR	C23-C22-C20	-2.38	108.43	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1203	OLC	C3-C2-C1	-2.26	105.42	113.69
7	B	102	MES	C7-N4-C5	2.20	117.10	111.24
4	A	1201	CLR	C8-C7-C6	-2.16	109.77	112.76
4	A	1202	CLR	C4-C5-C6	-2.15	117.66	120.57
4	A	1202	CLR	C21-C20-C17	-2.13	109.69	112.88
5	A	1204	OLC	C3-C2-C1	-2.09	106.02	113.69
4	A	1201	CLR	C21-C20-C17	2.08	116.00	112.88
7	B	102	MES	O2S-S-C8	2.06	109.84	106.73
5	A	1205	OLC	O20-C1-O19	-2.02	118.58	123.63
5	A	1204	OLC	O20-C1-O19	-2.02	118.59	123.63
5	A	1203	OLC	O20-C1-O19	-2.01	118.60	123.63

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1202	CLR	C13-C17-C20-C21
5	A	1204	OLC	C21-C22-C24-O25
7	B	102	MES	C8-C7-N4-C3
5	A	1205	OLC	O19-C1-O20-C21
4	A	1202	CLR	C13-C17-C20-C22
5	A	1205	OLC	C2-C1-O20-C21
4	A	1202	CLR	C16-C17-C20-C21
4	A	1202	CLR	C16-C17-C20-C22
5	A	1203	OLC	C2-C1-O20-C21
5	A	1203	OLC	O19-C1-O20-C21
4	A	1201	CLR	C17-C20-C22-C23
4	A	1201	CLR	C22-C23-C24-C25
4	A	1201	CLR	C21-C20-C22-C23
5	A	1205	OLC	O20-C21-C22-O23
4	A	1202	CLR	C20-C22-C23-C24
5	A	1203	OLC	C21-C22-C24-O25
5	A	1204	OLC	O23-C22-C24-O25
4	A	1201	CLR	C23-C24-C25-C26
5	A	1204	OLC	C2-C1-O20-C21
5	A	1206	OLC	C12-C13-C14-C15
5	A	1204	OLC	O19-C1-O20-C21
5	A	1203	OLC	C7-C8-C9-C10
5	A	1203	OLC	C10-C11-C12-C13
5	A	1203	OLC	C2-C3-C4-C5
4	A	1201	CLR	C23-C24-C25-C27
7	B	102	MES	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
5	A	1204	OLC	C6-C7-C8-C9
5	A	1203	OLC	C4-C5-C6-C7
5	A	1205	OLC	C14-C15-C16-C17
7	B	102	MES	N4-C7-C8-S
5	A	1203	OLC	O20-C21-C22-O23
5	A	1205	OLC	C2-C3-C4-C5
5	A	1203	OLC	C14-C15-C16-C17
4	A	1201	CLR	C16-C17-C20-C22
5	A	1203	OLC	C3-C4-C5-C6
5	A	1203	OLC	C15-C16-C17-C18
5	A	1203	OLC	O23-C22-C24-O25
5	A	1203	OLC	C11-C12-C13-C14
5	A	1204	OLC	C2-C3-C4-C5

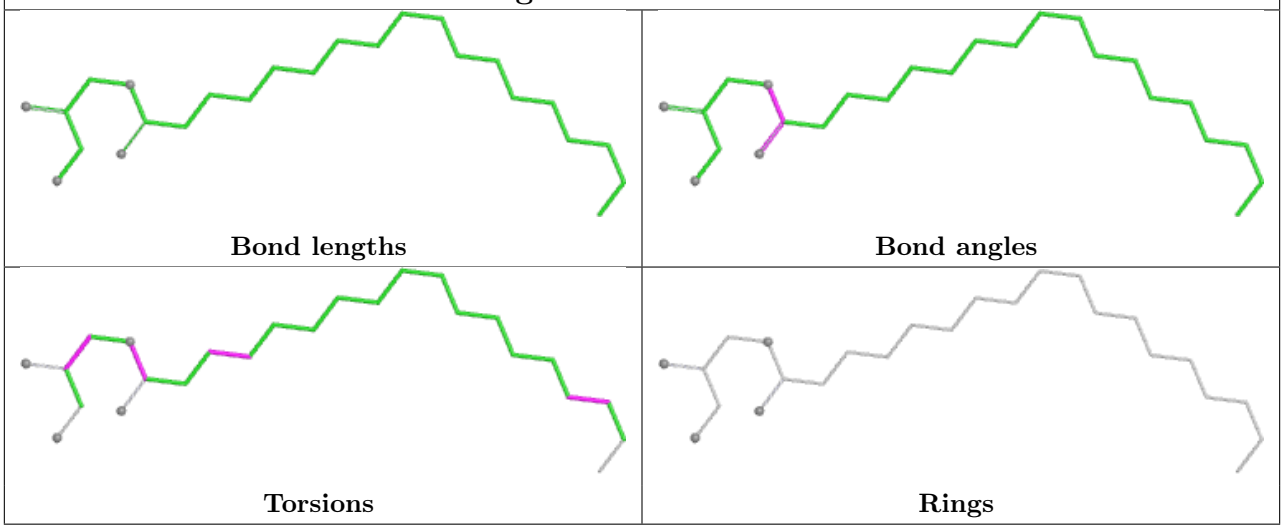
There are no ring outliers.

6 monomers are involved in 17 short contacts:

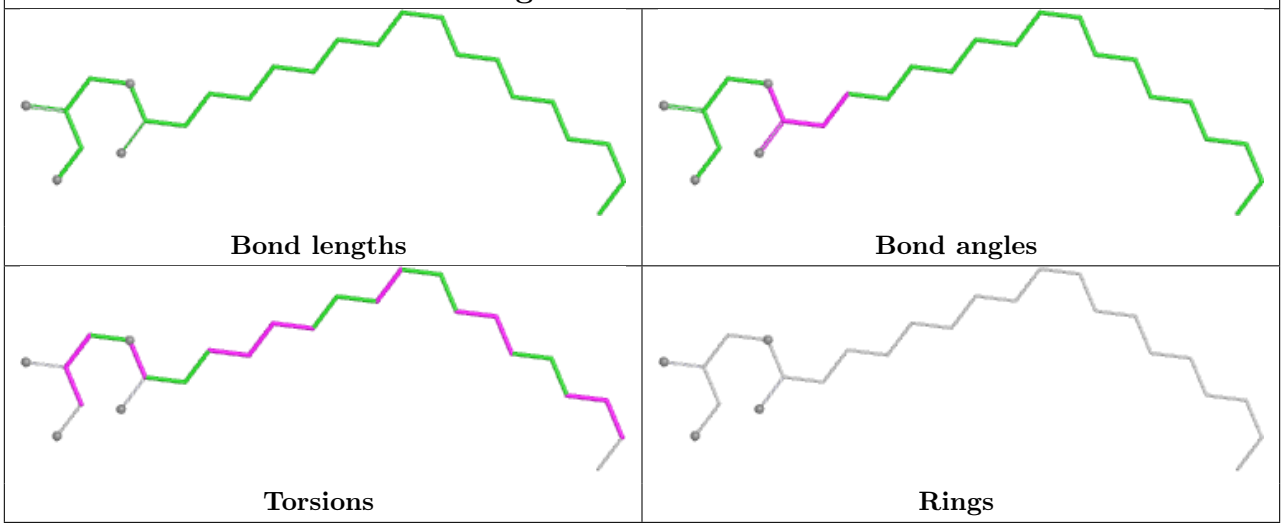
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1203	OLC	1	0
4	A	1202	CLR	4	0
7	B	102	MES	5	0
5	A	1206	OLC	2	0
4	A	1201	CLR	4	0
5	A	1204	OLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

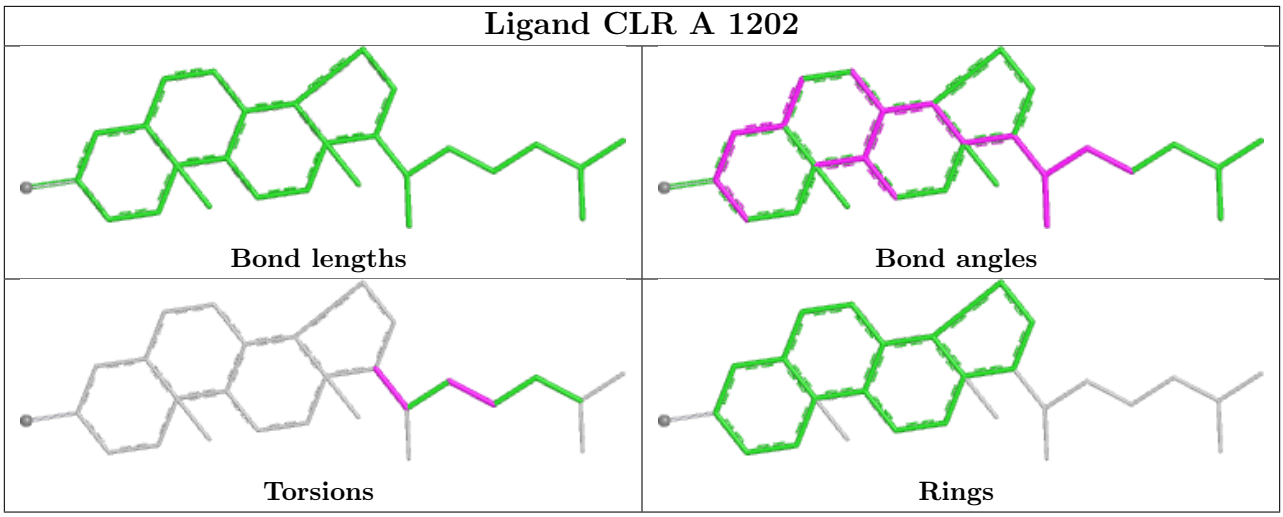
Ligand OLC A 1205

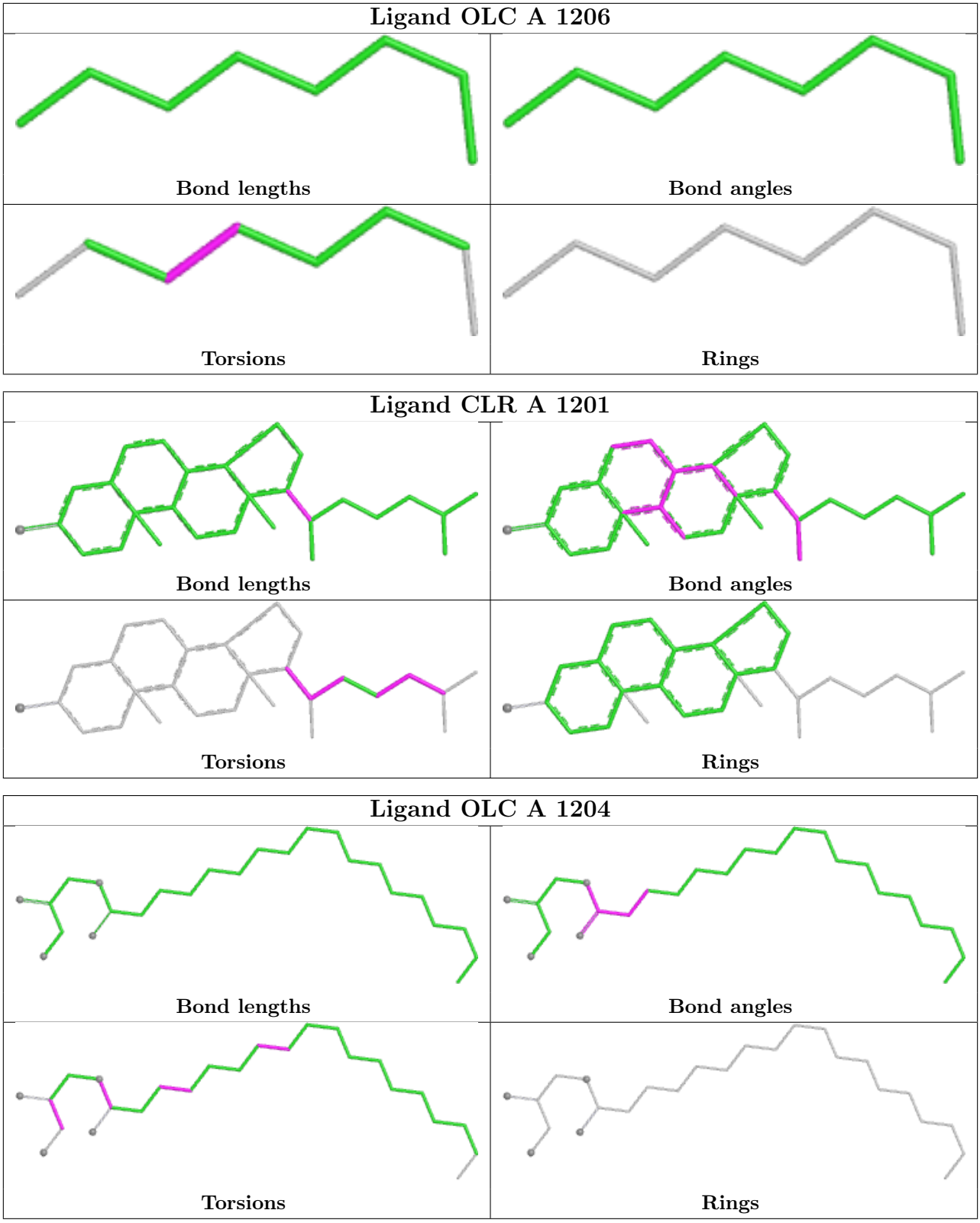


Ligand OLC A 1203



Ligand CLR A 1202





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	419/460 (91%)	0.13	8 (1%)	66	41	48, 73, 109, 152	0
2	B	73/76 (96%)	0.34	2 (2%)	56	33	60, 100, 126, 129	0
3	D	126/131 (96%)	0.29	1 (0%)	82	60	78, 106, 133, 142	0
All	All	618/667 (92%)	0.18	11 (1%)	67	42	48, 84, 123, 152	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	35	GLY	2.6
1	A	178	ASP	2.5
2	B	34	CYS	2.3
1	A	170	ASP	2.3
1	A	176	ASP	2.3
1	A	157	ILE	2.2
1	A	1052	THR	2.2
1	A	1033	ALA	2.2
3	D	28	SER	2.2
1	A	167	THR	2.2
1	A	1051	ILE	2.1

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

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	PCA	D	1	8/9	0.46	0.15	120,128,133,135	0
1	YCM	A	304	10/11	0.76	0.10	75,100,112,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	YCM	A	66	10/11	0.87	0.12	62,79,85,92	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

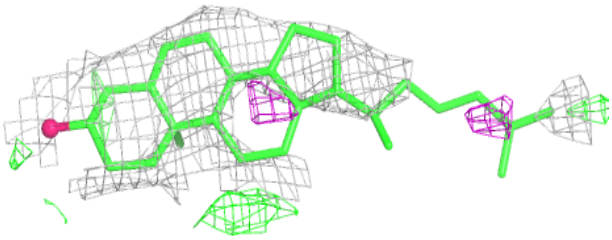
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

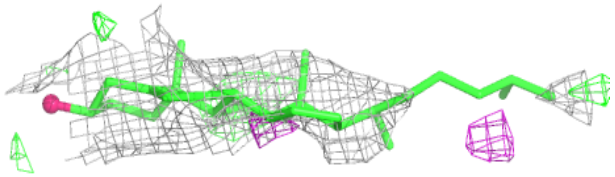
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CLR	A	1202	28/28	0.60	0.23	64,103,118,124	0
4	CLR	A	1201	28/28	0.65	0.21	62,110,123,124	0
5	OLC	A	1203	25/25	0.75	0.17	44,63,89,99	0
5	OLC	A	1206	8/25	0.77	0.23	66,74,82,83	0
5	OLC	A	1205	25/25	0.82	0.16	42,77,93,116	0
5	OLC	A	1204	25/25	0.84	0.15	60,83,105,108	0
7	MES	B	102	12/12	0.84	0.17	87,106,111,116	0
6	ZN	B	101	1/1	0.96	0.07	101,101,101,101	0

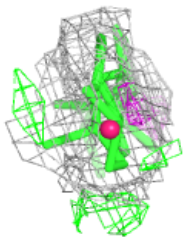
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLR A 1202:

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

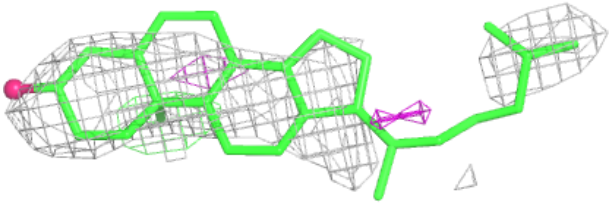


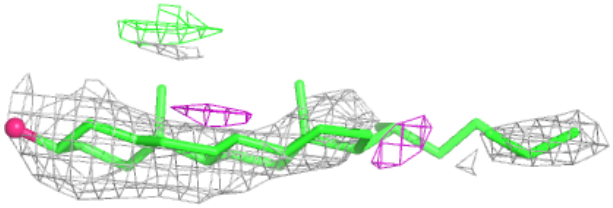


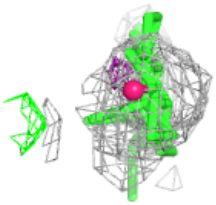


Electron density around CLR A 1201:

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

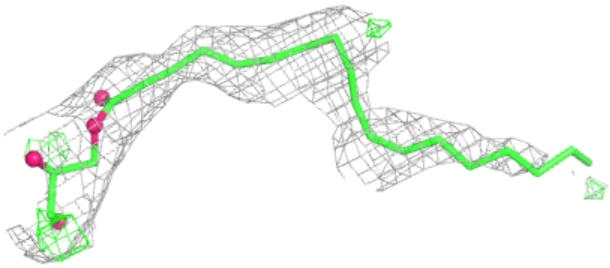


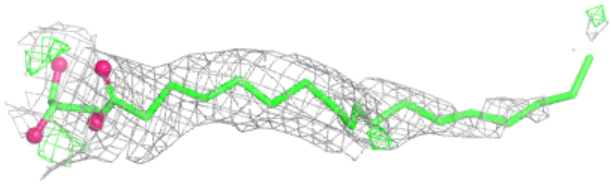


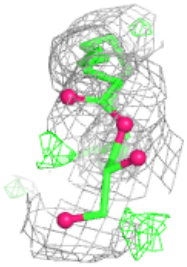


Electron density around OLC A 1203:

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

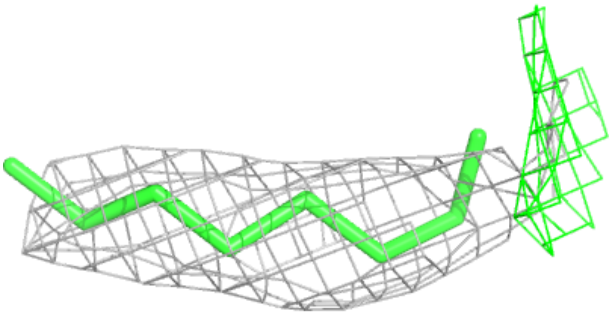


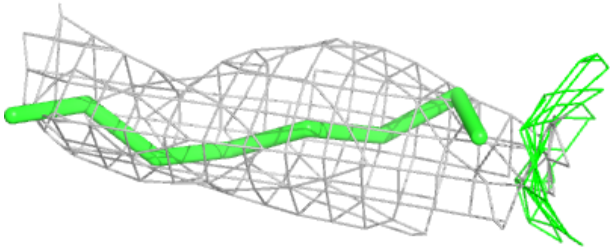


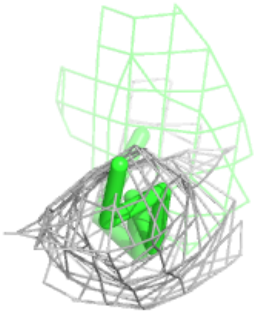


Electron density around OLC A 1206:

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

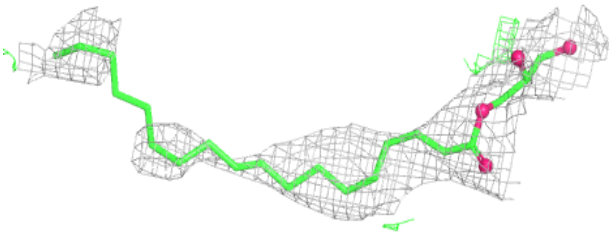


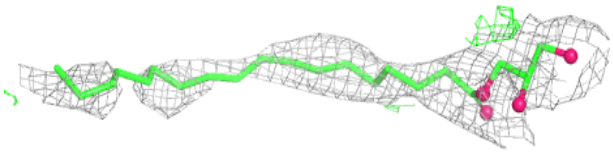


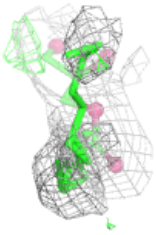


Electron density around OLC A 1205:

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







Electron density around OLC A 1204:

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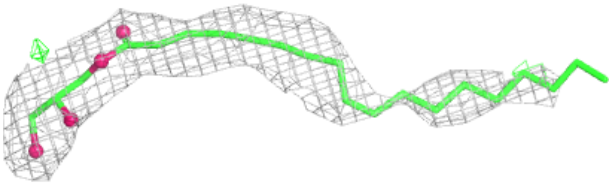
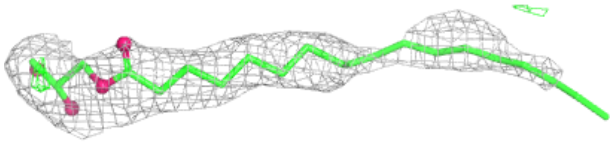
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.