wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 01:25 AM EST

PDB ID	:	7SK3
EMDB ID	:	EMD-25171
Title	:	Cryo-EM structure of ACKR3 in complex with CXCL12, an intracellular Fab, and an extracellular Fab
Authors	:	Yen, Y.C.; Schafer, C.T.; Gustavsson, M.; Handel, T.M.; Tesmer, J.J.G.
Deposited on	:	2021-10-19
Resolution	:	3.80 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp
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:

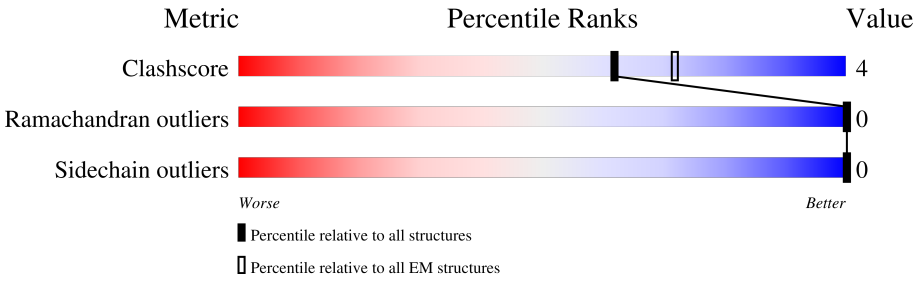
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	393	71% 7% 23%
2	B	68	87% 13%
3	C	215	41% 8% 51%
4	D	236	45% 7% 48%
5	E	215	47% · 51%
6	F	238	46% 6% 47%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13662 atoms, of which 6859 are hydrogens and 0 are deuteriums.

In the tables below, 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 Atypical chemokine receptor 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	304	4967	1636	2507	389	414	21	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP P25106
A	0	ALA	-	cloning artifact	UNP P25106
A	1	PRO	-	cloning artifact	UNP P25106
A	363	GLY	-	expression tag	UNP P25106
A	364	ARG	-	expression tag	UNP P25106
A	365	PRO	-	expression tag	UNP P25106
A	366	LEU	-	expression tag	UNP P25106
A	367	GLU	-	expression tag	UNP P25106
A	368	VAL	-	expression tag	UNP P25106
A	369	LEU	-	expression tag	UNP P25106
A	370	PHE	-	expression tag	UNP P25106
A	371	GLN	-	expression tag	UNP P25106
A	372	GLY	-	expression tag	UNP P25106
A	373	PRO	-	expression tag	UNP P25106
A	374	HIS	-	expression tag	UNP P25106
A	375	HIS	-	expression tag	UNP P25106
A	376	HIS	-	expression tag	UNP P25106
A	377	HIS	-	expression tag	UNP P25106
A	378	HIS	-	expression tag	UNP P25106
A	379	HIS	-	expression tag	UNP P25106
A	380	HIS	-	expression tag	UNP P25106
A	381	HIS	-	expression tag	UNP P25106
A	382	HIS	-	expression tag	UNP P25106
A	383	HIS	-	expression tag	UNP P25106
A	384	ASP	-	expression tag	UNP P25106
A	385	TYR	-	expression tag	UNP P25106
A	386	LYS	-	expression tag	UNP P25106
A	387	ASP	-	expression tag	UNP P25106

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Chain	Residue	Modelled	Actual	Comment	Reference
A	388	ASP	-	expression tag	UNP P25106
A	389	ASP	-	expression tag	UNP P25106
A	390	ASP	-	expression tag	UNP P25106
A	391	LYS	-	expression tag	UNP P25106

- Molecule 2 is a protein called Stromal cell-derived factor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	68	Total	C	H	N	O	S	0	0
			1145	356	586	106	93	4		

- Molecule 3 is a protein called CID25 Fab light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	105	Total	C	H	N	O	S	0	0
			1592	514	784	131	160	3		

- Molecule 4 is a protein called CID25 Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	123	Total	C	H	N	O	S	0	0
			1888	631	913	159	182	3		

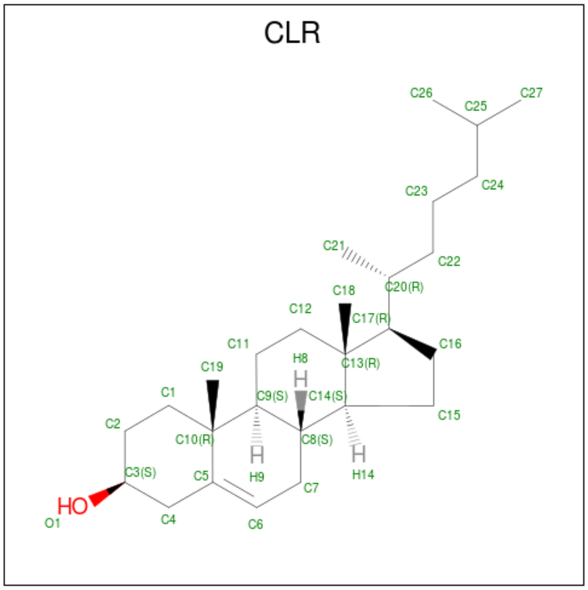
- Molecule 5 is a protein called CID24 Fab light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	106	Total	C	H	N	O	S	0	0
			1607	514	795	133	162	3		

- Molecule 6 is a protein called CID24 Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	125	Total	C	H	N	O	S	0	0
			1871	613	906	161	187	4		

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



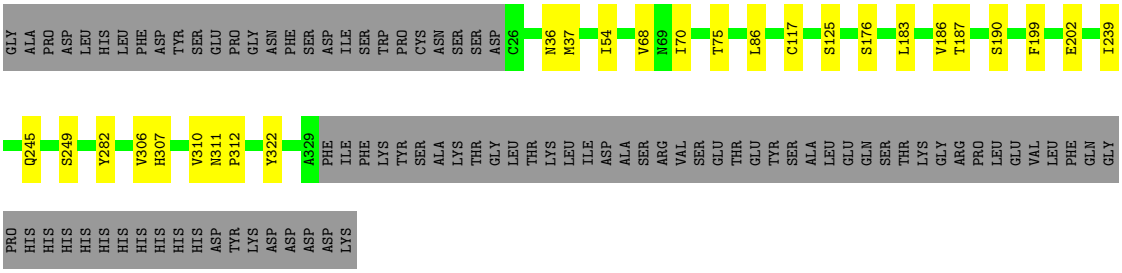
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
7	A	1	592	216	368	8	0
7	A	1	592	216	368	8	0
7	A	1	592	216	368	8	0
7	A	1	592	216	368	8	0
7	A	1	592	216	368	8	0
7	A	1	592	216	368	8	0
7	A	1	592	216	368	8	0
7	A	1	592	216	368	8	0

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. 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. 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.

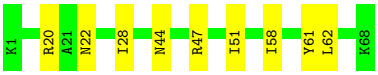
- Molecule 1: Atypical chemokine receptor 3

Chain A:



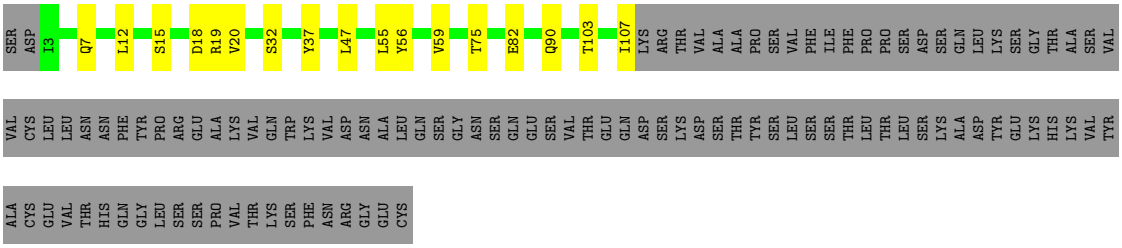
- Molecule 2: Stromal cell-derived factor 1

Chain B:



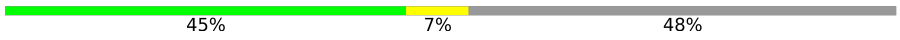
- Molecule 3: CID25 Fab light chain

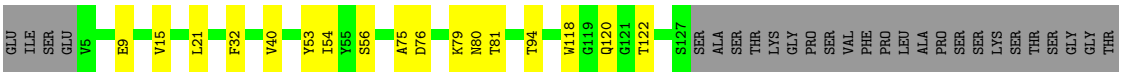
Chain C:

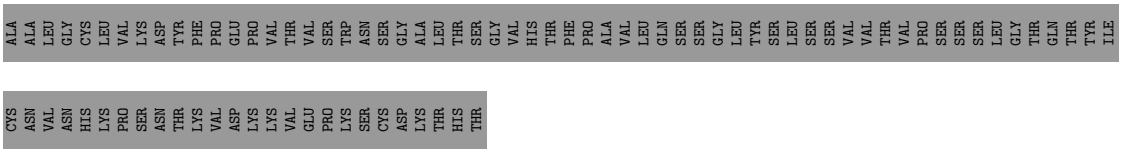


- Molecule 4: CID25 Fab heavy chain

Chain D:

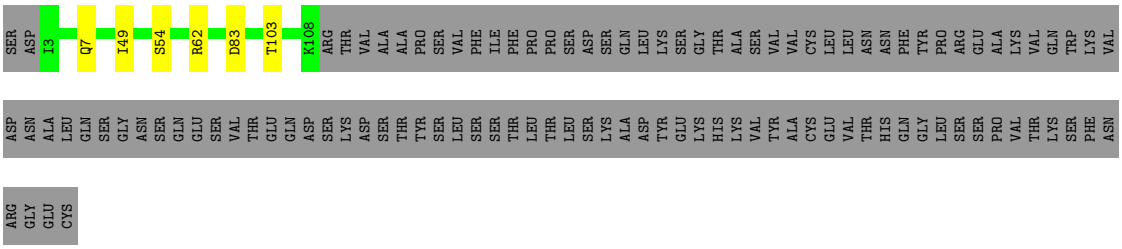






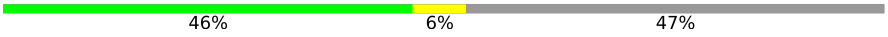
• Molecule 5: CID24 Fab light chain

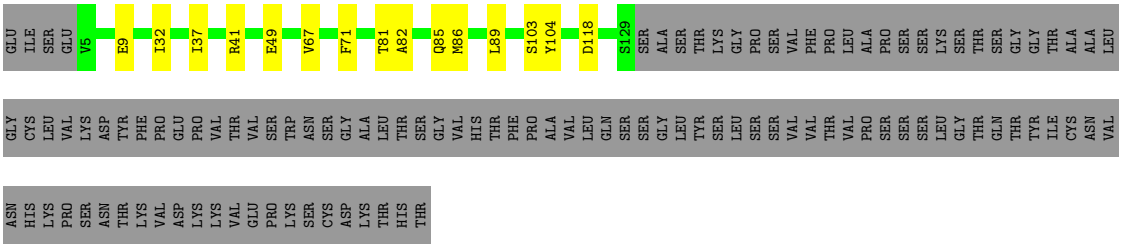
Chain E:



• Molecule 6: CID24 Fab heavy chain

Chain F:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	528797	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.25	0/2531	0.42	0/3460
2	B	0.27	0/570	0.48	0/767
3	C	0.27	0/828	0.50	0/1125
4	D	0.29	0/1007	0.48	0/1373
5	E	0.27	0/831	0.48	0/1128
6	F	0.26	0/993	0.49	0/1353
All	All	0.26	0/6760	0.46	0/9206

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	2460	2507	2507	18	0
2	B	559	586	587	5	0
3	C	808	784	785	13	0
4	D	975	913	912	11	0
5	E	812	795	794	3	0
6	F	965	906	906	11	0
7	A	224	368	368	4	0
All	All	6803	6859	6859	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 4.

The worst 5 of 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)
2:B:22:ASN:ND2	2:B:44:ASN:OD1	2.28	0.67
1:A:75:THR:HG22	1:A:75:THR:O	2.02	0.59
7:A:605:CLR:H212	7:A:605:CLR:H183	1.85	0.57
1:A:190:SER:O	4:D:53:TYR:OH	2.23	0.55
3:C:82:GLU:N	3:C:82:GLU:OE1	2.40	0.54

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 PDB entries followed by that with respect to all EM entries.

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	302/393 (77%)	296 (98%)	6 (2%)	0	100	100
2	B	66/68 (97%)	61 (92%)	5 (8%)	0	100	100
3	C	103/215 (48%)	91 (88%)	12 (12%)	0	100	100
4	D	121/236 (51%)	114 (94%)	7 (6%)	0	100	100
5	E	104/215 (48%)	101 (97%)	3 (3%)	0	100	100
6	F	123/238 (52%)	115 (94%)	8 (6%)	0	100	100
All	All	819/1365 (60%)	778 (95%)	41 (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 PDB entries followed by that with respect to all EM

entries.

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	283/363 (78%)	283 (100%)	0	100	100
2	B	63/63 (100%)	63 (100%)	0	100	100
3	C	91/190 (48%)	91 (100%)	0	100	100
4	D	99/198 (50%)	99 (100%)	0	100	100
5	E	92/190 (48%)	92 (100%)	0	100	100
6	F	101/200 (50%)	101 (100%)	0	100	100
All	All	729/1204 (60%)	729 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\|>2$
7	CLR	A	602	-	31,31,31	1.04	1 (3%)	48,48,48	1.33	7 (14%)
7	CLR	A	605	-	31,31,31	1.05	1 (3%)	48,48,48	1.34	7 (14%)
7	CLR	A	604	-	31,31,31	1.04	1 (3%)	48,48,48	1.32	8 (16%)
7	CLR	A	608	-	31,31,31	1.05	2 (6%)	48,48,48	1.33	9 (18%)
7	CLR	A	603	-	31,31,31	1.02	1 (3%)	48,48,48	1.32	7 (14%)
7	CLR	A	606	-	31,31,31	1.04	0	48,48,48	1.31	6 (12%)
7	CLR	A	607	-	31,31,31	1.05	2 (6%)	48,48,48	1.34	7 (14%)
7	CLR	A	601	-	31,31,31	1.04	1 (3%)	48,48,48	1.31	5 (10%)

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
7	CLR	A	602	-	-	2/10/68/68	0/4/4/4
7	CLR	A	605	-	-	6/10/68/68	0/4/4/4
7	CLR	A	604	-	-	3/10/68/68	0/4/4/4
7	CLR	A	608	-	-	3/10/68/68	0/4/4/4
7	CLR	A	603	-	-	2/10/68/68	0/4/4/4
7	CLR	A	606	-	-	1/10/68/68	0/4/4/4
7	CLR	A	607	-	-	3/10/68/68	0/4/4/4
7	CLR	A	601	-	-	5/10/68/68	0/4/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	605	CLR	C18-C13	-2.21	1.50	1.54
7	A	602	CLR	C18-C13	-2.21	1.50	1.54
7	A	608	CLR	C18-C13	-2.14	1.50	1.54
7	A	601	CLR	C18-C13	-2.13	1.50	1.54
7	A	603	CLR	C18-C13	-2.07	1.50	1.54

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	601	CLR	C22-C20-C17	-3.22	103.62	110.28
7	A	603	CLR	C22-C20-C17	-3.11	103.86	110.28
7	A	602	CLR	C22-C20-C17	-3.08	103.91	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	608	CLR	C22-C20-C17	-3.05	103.99	110.28
7	A	606	CLR	C12-C13-C14	-3.00	102.62	107.27

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	605	CLR	C16-C17-C20-C22
7	A	604	CLR	C17-C20-C22-C23
7	A	604	CLR	C21-C20-C22-C23
7	A	605	CLR	C13-C17-C20-C21
7	A	605	CLR	C17-C20-C22-C23

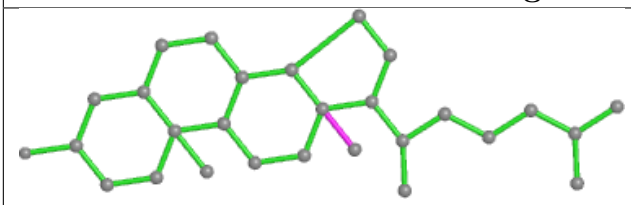
There are no ring outliers.

3 monomers are involved in 4 short contacts:

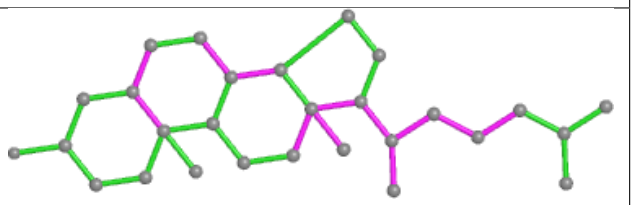
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	605	CLR	1	0
7	A	604	CLR	1	0
7	A	607	CLR	2	0

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.

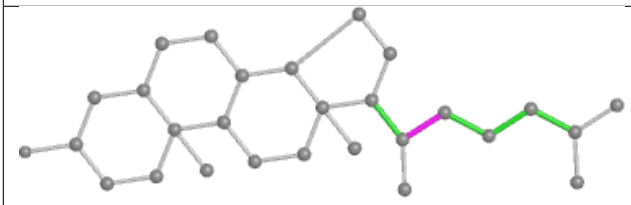
Ligand CLR A 602



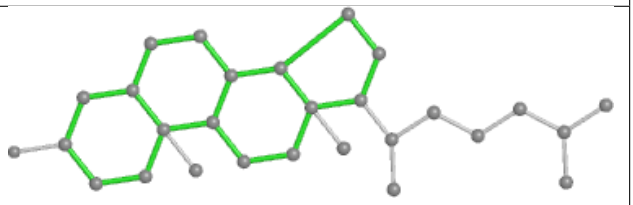
Bond lengths



Bond angles

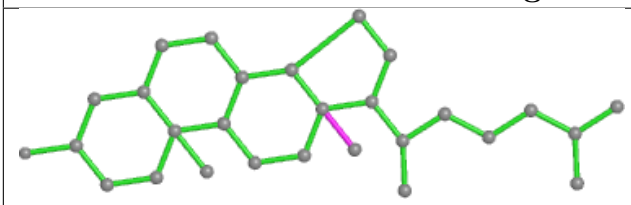


Torsions

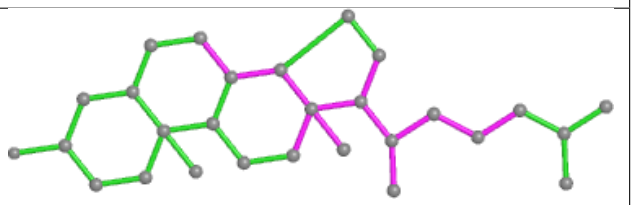


Rings

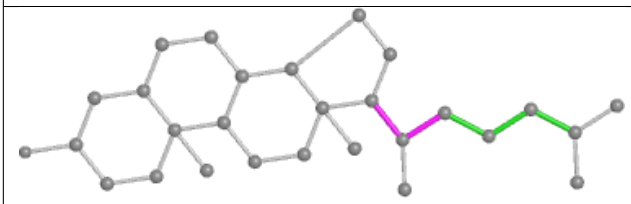
Ligand CLR A 605



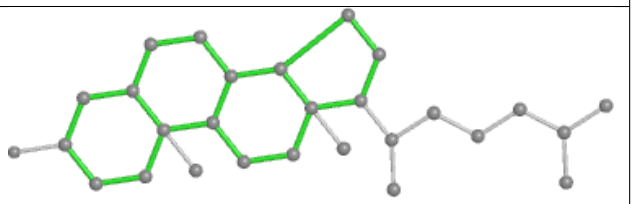
Bond lengths



Bond angles

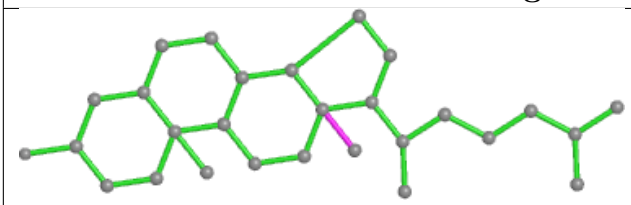


Torsions

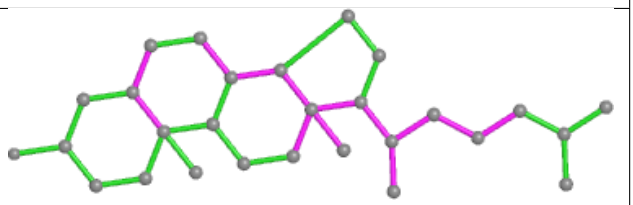


Rings

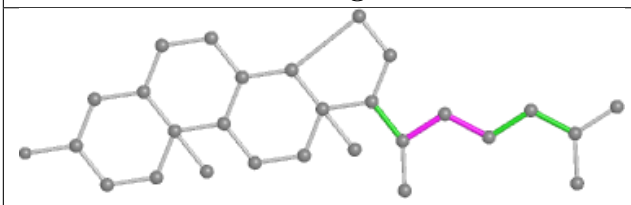
Ligand CLR A 604



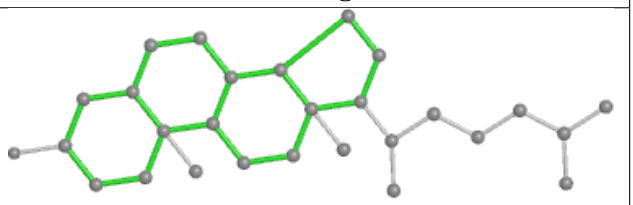
Bond lengths



Bond angles

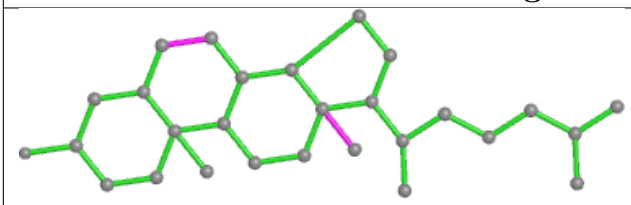


Torsions

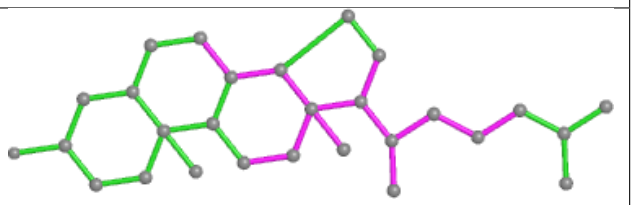


Rings

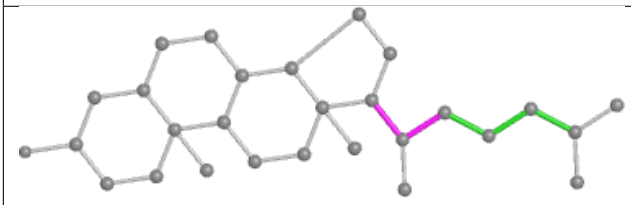
Ligand CLR A 608



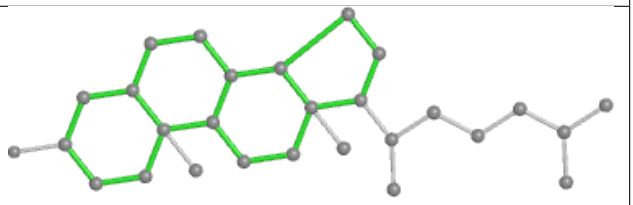
Bond lengths



Bond angles

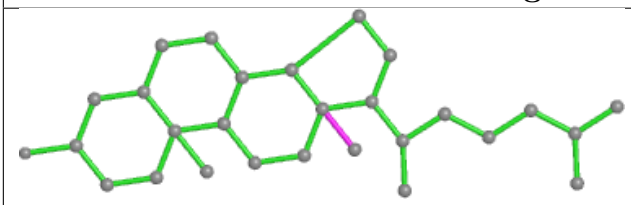


Torsions

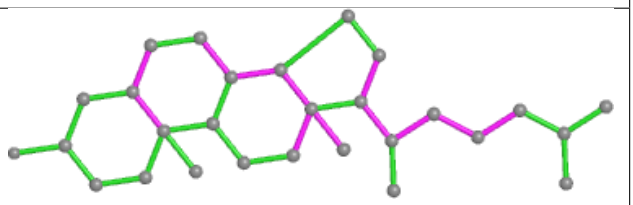


Rings

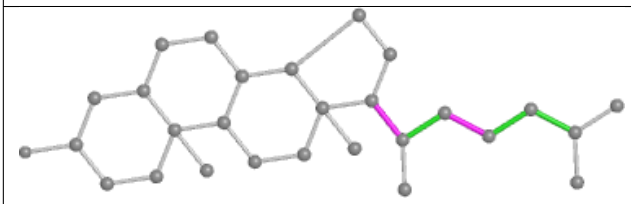
Ligand CLR A 603



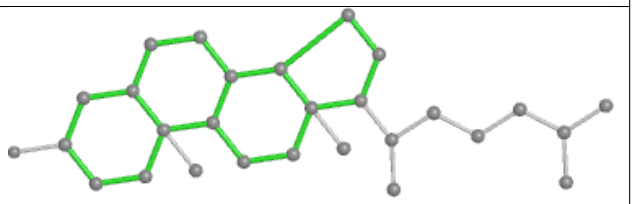
Bond lengths



Bond angles

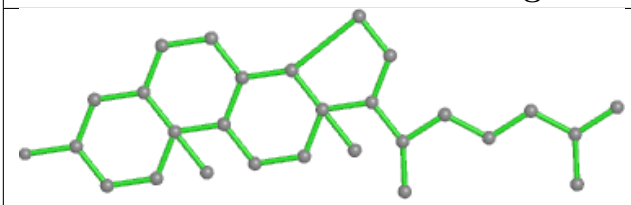


Torsions

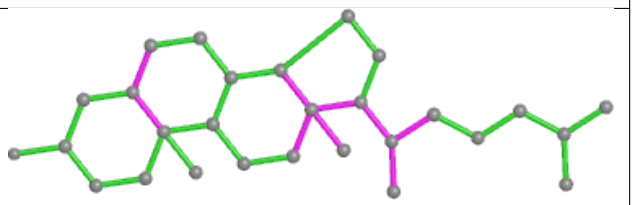


Rings

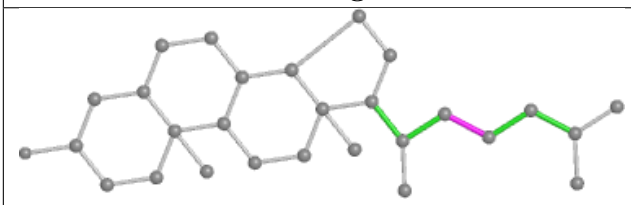
Ligand CLR A 606



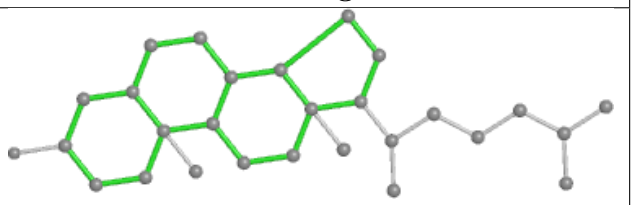
Bond lengths



Bond angles

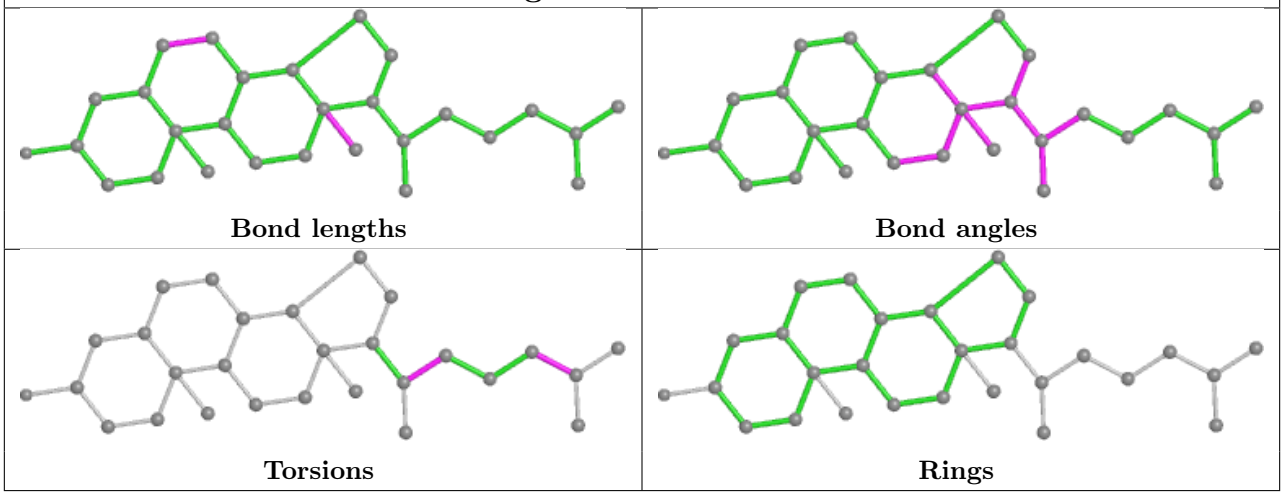


Torsions

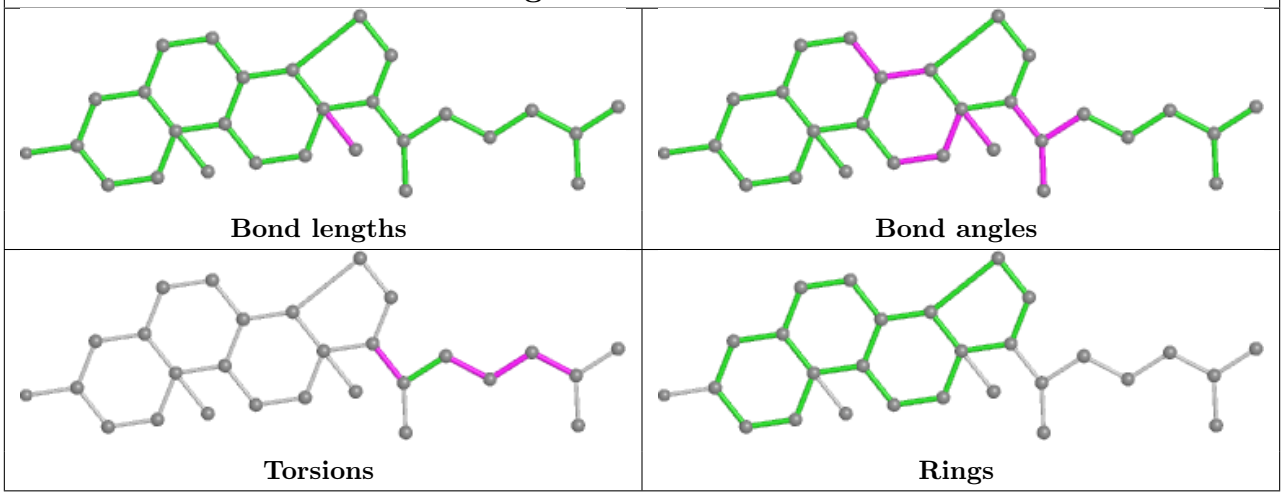


Rings

Ligand CLR A 607



Ligand CLR A 601



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 Map visualisation

This section contains visualisations of the EMDB entry EMD-25171. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.