



Full wwPDB EM Validation Report ⓘ

Nov 13, 2024 – 10:19 AM JST

PDB ID : 8YC0
EMDB ID : EMD-39128
Title : T cell receptor V delta2 V gamma9 in GDN
Authors : Xin, W.; Huang, B.; Chi, X.; Xu, M.; Zhang, Y.; Li, X.; Su, Q.; Zhou, Q.
Deposited on : 2024-02-17
Resolution : 4.12 Å(reported)

This is a Full wwPDB EM 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/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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

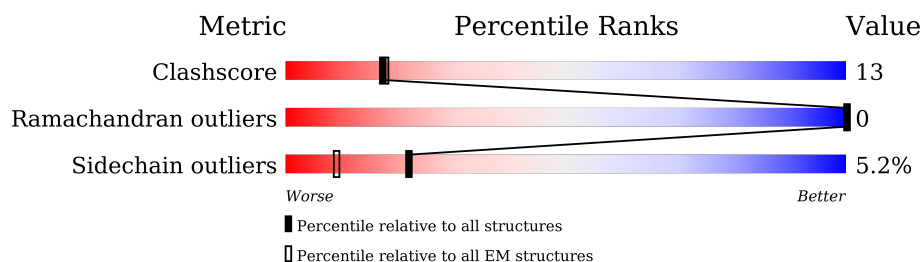
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.12 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	a	195	13% 87%
1	b	195	13% 86%
2	d	171	59% 39%
3	e	207	56% 42%
3	f	207	52% 43%
4	g	182	61% 37%
5	m	310	10% 89%
6	n	332	11% 89%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4635 atoms, of which 0 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 T-cell surface glycoprotein CD3 zeta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	26	Total	C	N	O	S	0	0
			203	142	27	33	1		
1	b	27	Total	C	N	O	S	0	0
			218	151	32	34	1		

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	165	ALA	-	expression tag	UNP P20963
a	166	ALA	-	expression tag	UNP P20963
a	167	ALA	-	expression tag	UNP P20963
a	168	TRP	-	expression tag	UNP P20963
a	169	SER	-	expression tag	UNP P20963
a	170	HIS	-	expression tag	UNP P20963
a	171	PRO	-	expression tag	UNP P20963
a	172	GLN	-	expression tag	UNP P20963
a	173	PHE	-	expression tag	UNP P20963
a	174	GLU	-	expression tag	UNP P20963
a	175	LYS	-	expression tag	UNP P20963
a	176	GLY	-	expression tag	UNP P20963
a	177	GLY	-	expression tag	UNP P20963
a	178	GLY	-	expression tag	UNP P20963
a	179	SER	-	expression tag	UNP P20963
a	180	GLY	-	expression tag	UNP P20963
a	181	GLY	-	expression tag	UNP P20963
a	182	GLY	-	expression tag	UNP P20963
a	183	SER	-	expression tag	UNP P20963
a	184	GLY	-	expression tag	UNP P20963
a	185	GLY	-	expression tag	UNP P20963
a	186	SER	-	expression tag	UNP P20963
a	187	ALA	-	expression tag	UNP P20963
a	188	TRP	-	expression tag	UNP P20963
a	189	SER	-	expression tag	UNP P20963
a	190	HIS	-	expression tag	UNP P20963

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
a	191	PRO	-	expression tag	UNP P20963
a	192	GLN	-	expression tag	UNP P20963
a	193	PHE	-	expression tag	UNP P20963
a	194	GLU	-	expression tag	UNP P20963
a	195	LYS	-	expression tag	UNP P20963
b	165	ALA	-	expression tag	UNP P20963
b	166	ALA	-	expression tag	UNP P20963
b	167	ALA	-	expression tag	UNP P20963
b	168	TRP	-	expression tag	UNP P20963
b	169	SER	-	expression tag	UNP P20963
b	170	HIS	-	expression tag	UNP P20963
b	171	PRO	-	expression tag	UNP P20963
b	172	GLN	-	expression tag	UNP P20963
b	173	PHE	-	expression tag	UNP P20963
b	174	GLU	-	expression tag	UNP P20963
b	175	LYS	-	expression tag	UNP P20963
b	176	GLY	-	expression tag	UNP P20963
b	177	GLY	-	expression tag	UNP P20963
b	178	GLY	-	expression tag	UNP P20963
b	179	SER	-	expression tag	UNP P20963
b	180	GLY	-	expression tag	UNP P20963
b	181	GLY	-	expression tag	UNP P20963
b	182	GLY	-	expression tag	UNP P20963
b	183	SER	-	expression tag	UNP P20963
b	184	GLY	-	expression tag	UNP P20963
b	185	GLY	-	expression tag	UNP P20963
b	186	SER	-	expression tag	UNP P20963
b	187	ALA	-	expression tag	UNP P20963
b	188	TRP	-	expression tag	UNP P20963
b	189	SER	-	expression tag	UNP P20963
b	190	HIS	-	expression tag	UNP P20963
b	191	PRO	-	expression tag	UNP P20963
b	192	GLN	-	expression tag	UNP P20963
b	193	PHE	-	expression tag	UNP P20963
b	194	GLU	-	expression tag	UNP P20963
b	195	LYS	-	expression tag	UNP P20963

- Molecule 2 is a protein called T-cell surface glycoprotein CD3 delta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	d	105	Total	C	N	O	S	0	0
			817	521	135	155	6		

- Molecule 3 is a protein called T-cell surface glycoprotein CD3 epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	121	Total	C	N	O	S	0	0
			959	609	151	191	8		
3	f	118	Total	C	N	O	S	0	0
			933	594	148	183	8		

- Molecule 4 is a protein called T-cell surface glycoprotein CD3 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	115	Total	C	N	O	S	0	0
			907	582	150	168	7		

- Molecule 5 is a protein called T cell receptor delta variable 2,T cell receptor delta constant.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	m	34	Total	C	N	O	S	0	0
			268	180	42	43	3		

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	-19	MET	-	initiating methionine	UNP A0JD36
m	-18	ASP	-	expression tag	UNP A0JD36
m	-17	MET	-	expression tag	UNP A0JD36
m	-16	ARG	-	expression tag	UNP A0JD36
m	-15	VAL	-	expression tag	UNP A0JD36
m	-14	PRO	-	expression tag	UNP A0JD36
m	-13	ALA	-	expression tag	UNP A0JD36
m	-12	GLN	-	expression tag	UNP A0JD36
m	-11	LEU	-	expression tag	UNP A0JD36
m	-10	LEU	-	expression tag	UNP A0JD36
m	-9	GLY	-	expression tag	UNP A0JD36
m	-8	LEU	-	expression tag	UNP A0JD36
m	-7	LEU	-	expression tag	UNP A0JD36
m	-6	LEU	-	expression tag	UNP A0JD36
m	-5	LEU	-	expression tag	UNP A0JD36
m	-4	TRP	-	expression tag	UNP A0JD36
m	-3	LEU	-	expression tag	UNP A0JD36
m	-2	SER	-	expression tag	UNP A0JD36
m	-1	GLY	-	expression tag	UNP A0JD36
m	0	ALA	-	expression tag	UNP A0JD36
m	1	ARG	-	expression tag	UNP A0JD36

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
m	2	CYS	-	expression tag	UNP A0JD36
m	3	MET	-	expression tag	UNP A0JD36
m	4	ASP	-	expression tag	UNP A0JD36
m	5	TYR	-	expression tag	UNP A0JD36
m	6	LYS	-	expression tag	UNP A0JD36
m	7	ASP	-	expression tag	UNP A0JD36
m	8	ASP	-	expression tag	UNP A0JD36
m	9	ASP	-	expression tag	UNP A0JD36
m	10	ASP	-	expression tag	UNP A0JD36
m	11	LYS	-	expression tag	UNP A0JD36
m	12	GLY	-	expression tag	UNP A0JD36
m	13	GLY	-	expression tag	UNP A0JD36
m	14	SER	-	expression tag	UNP A0JD36
m	15	GLU	-	expression tag	UNP A0JD36
m	16	THR	-	expression tag	UNP A0JD36
m	17	GLY	-	expression tag	UNP A0JD36
m	114	LEU	-	linker	UNP A0JD36
m	115	GLY	-	linker	UNP A0JD36
m	116	MET	-	linker	UNP A0JD36
m	117	GLY	-	linker	UNP A0JD36
m	118	GLY	-	linker	UNP A0JD36
m	119	GLU	-	linker	UNP A0JD36
m	120	TYR	-	linker	UNP A0JD36
m	121	THR	-	linker	UNP A0JD36
m	122	ASP	-	linker	UNP A0JD36
m	123	LYS	-	linker	UNP A0JD36
m	124	LEU	-	linker	UNP A0JD36
m	125	ILE	-	linker	UNP A0JD36
m	126	PHE	-	linker	UNP A0JD36
m	127	GLY	-	linker	UNP A0JD36
m	128	LYS	-	linker	UNP A0JD36
m	129	GLY	-	linker	UNP A0JD36
m	130	THR	-	linker	UNP A0JD36
m	131	ARG	-	linker	UNP A0JD36
m	132	VAL	-	linker	UNP A0JD36
m	133	THR	-	linker	UNP A0JD36
m	134	VAL	-	linker	UNP A0JD36
m	135	GLU	-	linker	UNP A0JD36
m	136	PRO	-	linker	UNP A0JD36
m	137	ARG	-	linker	UNP A0JD36

- Molecule 6 is a protein called T cell receptor gamma variable 9,T cell receptor gamma constant 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	n	37	Total	C	N	O	S	0	0
			302	203	46	50	3		

There are 57 discrepancies between the modelled and reference sequences:

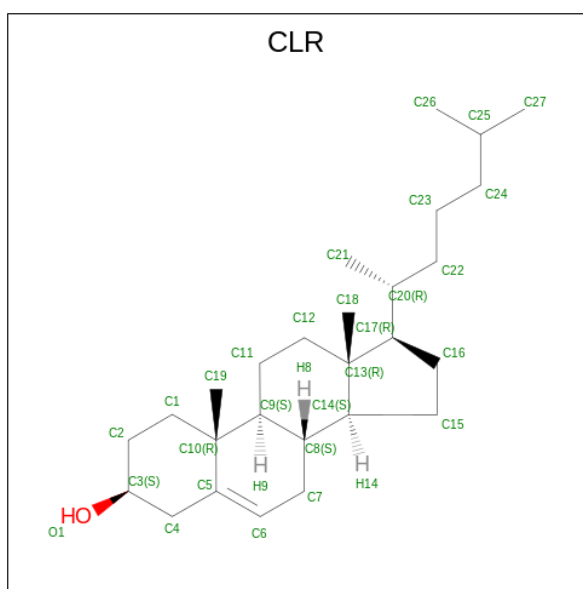
Chain	Residue	Modelled	Actual	Comment	Reference
n	-34	MET	-	initiating methionine	UNP Q99603
n	-33	ASP	-	expression tag	UNP Q99603
n	-32	MET	-	expression tag	UNP Q99603
n	-31	ARG	-	expression tag	UNP Q99603
n	-30	VAL	-	expression tag	UNP Q99603
n	-29	PRO	-	expression tag	UNP Q99603
n	-28	ALA	-	expression tag	UNP Q99603
n	-27	GLN	-	expression tag	UNP Q99603
n	-26	LEU	-	expression tag	UNP Q99603
n	-25	LEU	-	expression tag	UNP Q99603
n	-24	GLY	-	expression tag	UNP Q99603
n	-23	LEU	-	expression tag	UNP Q99603
n	-22	LEU	-	expression tag	UNP Q99603
n	-21	LEU	-	expression tag	UNP Q99603
n	-20	LEU	-	expression tag	UNP Q99603
n	-19	TRP	-	expression tag	UNP Q99603
n	-18	LEU	-	expression tag	UNP Q99603
n	-17	SER	-	expression tag	UNP Q99603
n	-16	GLY	-	expression tag	UNP Q99603
n	-15	ALA	-	expression tag	UNP Q99603
n	-14	ARG	-	expression tag	UNP Q99603
n	-13	CYS	-	expression tag	UNP Q99603
n	-12	MET	-	expression tag	UNP Q99603
n	-11	ASP	-	expression tag	UNP Q99603
n	-10	TYR	-	expression tag	UNP Q99603
n	-9	LYS	-	expression tag	UNP Q99603
n	-8	ASP	-	expression tag	UNP Q99603
n	-7	ASP	-	expression tag	UNP Q99603
n	-6	ASP	-	expression tag	UNP Q99603
n	-5	ASP	-	expression tag	UNP Q99603
n	-4	LYS	-	expression tag	UNP Q99603
n	-3	GLY	-	expression tag	UNP Q99603
n	-2	GLY	-	expression tag	UNP Q99603
n	-1	SER	-	expression tag	UNP Q99603
n	0	GLU	-	expression tag	UNP Q99603
n	1	THR	-	expression tag	UNP Q99603
n	104	ALA	-	linker	UNP Q99603

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
n	105	GLN	-	linker	UNP Q99603
n	106	GLN	-	linker	UNP Q99603
n	107	GLU	-	linker	UNP Q99603
n	108	LEU	-	linker	UNP Q99603
n	109	GLY	-	linker	UNP Q99603
n	110	LYS	-	linker	UNP Q99603
n	111	LYS	-	linker	UNP Q99603
n	112	ILE	-	linker	UNP Q99603
n	113	LYS	-	linker	UNP Q99603
n	114	VAL	-	linker	UNP Q99603
n	115	PHE	-	linker	UNP Q99603
n	116	GLY	-	linker	UNP Q99603
n	117	PRO	-	linker	UNP Q99603
n	118	GLY	-	linker	UNP Q99603
n	119	THR	-	linker	UNP Q99603
n	120	LYS	-	linker	UNP Q99603
n	121	LEU	-	linker	UNP Q99603
n	122	ILE	-	linker	UNP Q99603
n	123	ILE	-	linker	UNP Q99603
n	124	THR	-	linker	UNP Q99603

- 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
7	b	1	Total	C	O	0
			28	27	1	

GLY
GLY
ARG
GLN
GLY
ARG
GLY
GLN
ASN
LYS
GLU
ARG
PRO
PRO
PRO
VAL
SER
PRO
ASN
PRO
TYR
GLU
PRO
ILE
ILE
ARG
LYS
GLY
GLN
ARG
LEU
ASP
LEU
TYR
SER
GLY
ASN
GLN
ARG
ILE

- Molecule 3: T-cell surface glycoprotein CD3 epsilon chain

Chain f: 52% 43%

MET
GLN
SER
GLY
THR
HIS
TRP
ARG
VAL
LEU
LEU
LEU
CYS
LEU
LEU
SER
SER
VAL
GLY
GLN
VAL
TRP
GLY
ASP
GLN
ASP
ASN
ASN
GLU
ARG
MET
GLY
PRO
GLY
ILE
THR
Q33
C49
K64
D69
ASP
ASP
LYS
W74
F87
C98
F110
L114
C119
E120
N121
M125
D137

- Molecule 4: T-cell surface glycoprotein CD3 gamma chain

Chain g: 61% 37%

MET
GLU
GLN
GLY
LYS
GLY
LEU
ALA
VAL
LEU
LEU
ILE
LEU
ALA
ILE
ILE
LEU
LEU
GLN
GLY
THR
ALA
GLN
SER
ILE
K26
D39
L65
D80
N92
D140
GLY
VAL
ARG
GLN
SER
SER
ALA
SER
ASP
LYS
THR
LEU
PRO
ASN
ASP
GLN
ARG
ILE

- Molecule 5: T cell receptor delta variable 2,T cell receptor delta constant

Chain m: 10% 89%

MET
ASP
MET
MET
VAL
PRO
ALA
GLN
LEU
LEU
LEU
LEU
LEU
LEU
LEU
TRP
SER
GLY
ALA
ARG
MET
CYS
MET
ASP
TYR
LYS
ASP
ASP
LYS
GLY
SER
GLY
THR
GLY
ALA
ILE
ASP
PHE
LEU
LEU
GLN
PHE
ASP
GLN
PHE
LEU
VAL
PRO
GLY
HIS
GLU
THR
VAL
SER
ILE
VAL
VAL
PRO
THR
LEU
ARG
CYS

- Molecule 6: T cell receptor gamma variable 9,T cell receptor gamma constant 1

Chain n: 11% 89%

MET
ASP
MET
MET
VAL
PRO
ALA
GLN
LEU
LEU
LEU
LEU
LEU
TRP
GLU
SER
GLY
ALA
ARG
GLY
ARG
GLN
GLN
GLU
VAL
VAL
ILE
MET
CYS
MET
ASP
TYR
LYS
ASP
ASP
GLY
GLY
SER
THR
VAL
VAL
ARG
LYS
GLY
ALA
GLY
HIS
LEU
LEU
GLN
PRO
GLY
PRO
GLN
ILE
SER
SER
VAL
SER
PRO
LYS
THR
THR
LEU
SER
GLU
PHE
ILE
THR
SER
PRO
SER
ARG
ALA
THR
LEU
LEU
ALA
CYS

THR	THR
LYS	LYS
LEU	LEU
GLN	GLN
LYS	HIS
ALA	ARG
GLY	CYS
THR	ILE
TYR	VAL
LEU	ARG
CYS	HIS
LEU	GLU
LEU	ASN
GLU	ASN
LYS	LYS
PHE	ASN
PHE	GLY
PRO	VAL
ASP	ASP
VAL	GLN
ILE	GLU
LYS	ILE
ILE	ILE
HIS	PHE
TRP	PRO
GLN	PRO
GLU	ILE
LYS	LYS
LYS	THR
SER	ASP
ASN	VAL
THR	ILE
ILE	THR
LEU	MET
GLY	ASP
SER	PRO
GLN	LYS
GLU	ASP
GLY	ASN
THR	CYS
MET	SER
LYS	LYS
THR	ASP
ALA	ALA
ASN	ASN
ASP	ASP
THR	T252
TYR	T288
MET	ALA
LYS	PHE
PHE	CYS
SER	CYS
TRP	ASN
LEU	ASN
THR	GLY
VAL	GLU
PRO	LYS
GLU	SER
LYS	
SER	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119724	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (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	0.29	0/207	0.52	0/281
1	b	0.29	0/222	0.44	0/300
2	d	0.25	0/829	0.57	0/1127
3	e	0.27	0/980	0.59	0/1331
3	f	0.27	0/953	0.57	3/1294 (0.2%)
4	g	0.27	0/925	0.53	1/1244 (0.1%)
5	m	0.30	0/271	0.60	0/363
6	n	0.30	0/306	0.50	0/416
All	All	0.27	0/4693	0.56	4/6356 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	f	114	LEU	CA-CB-CG	6.02	129.15	115.30
4	g	39	ASP	CB-CG-OD2	5.62	123.36	118.30
3	f	137	ASP	CB-CG-OD1	5.50	123.25	118.30
3	f	49	CYS	CA-CB-SG	5.08	123.14	114.00

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	203	0	218	0	0
1	b	218	0	239	0	0
2	d	817	0	828	0	0
3	e	959	0	919	0	0
3	f	933	0	897	0	0
4	g	907	0	897	0	0
5	m	268	0	296	0	0
6	n	302	0	332	0	0
7	b	28	0	46	0	0
All	All	4635	0	4672	0	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 13.

There are no clashes within the asymmetric unit.

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	24/195 (12%)	21 (88%)	3 (12%)	0	100	100
1	b	25/195 (13%)	25 (100%)	0	0	100	100
2	d	103/171 (60%)	94 (91%)	9 (9%)	0	100	100
3	e	119/207 (58%)	108 (91%)	11 (9%)	0	100	100
3	f	114/207 (55%)	105 (92%)	9 (8%)	0	100	100
4	g	113/182 (62%)	102 (90%)	11 (10%)	0	100	100
5	m	32/310 (10%)	32 (100%)	0	0	100	100
6	n	35/332 (10%)	35 (100%)	0	0	100	100
All	All	565/1799 (31%)	522 (92%)	43 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	22/154 (14%)	21 (96%)	1 (4%)	23	47
1	b	24/154 (16%)	22 (92%)	2 (8%)	9	30
2	d	93/147 (63%)	89 (96%)	4 (4%)	25	48
3	e	109/177 (62%)	103 (94%)	6 (6%)	18	42
3	f	106/177 (60%)	98 (92%)	8 (8%)	11	33
4	g	97/155 (63%)	93 (96%)	4 (4%)	26	49
5	m	30/272 (11%)	28 (93%)	2 (7%)	13	36
6	n	35/298 (12%)	35 (100%)	0	100	100
All	All	516/1534 (34%)	489 (95%)	27 (5%)	22	43

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	26	LEU
1	b	40	PHE
1	b	54	LYS
2	d	37	CYS
2	d	66	ASP
2	d	91	ARG
2	d	125	PHE
3	e	62	ASN
3	e	78	ASP
3	e	87	PHE
3	e	114	LEU
3	e	122	CYS
3	e	153	LYS
3	f	49	CYS
3	f	64	LYS
3	f	87	PHE
3	f	98	CYS
3	f	110	PHE
3	f	119	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	f	121	ASN
3	f	125	MET
4	g	39	ASP
4	g	65	LEU
4	g	80	ASP
4	g	92	ASN
5	m	258	LYS
5	m	288	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	d	36	ASN
2	d	87	GLN
4	g	86	GLN
6	n	259	ASN

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](#)

1 ligand is 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	b	201	-	31,31,31	0.26	0	48,48,48	0.41	0

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	b	201	-	-	4/10/68/68	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

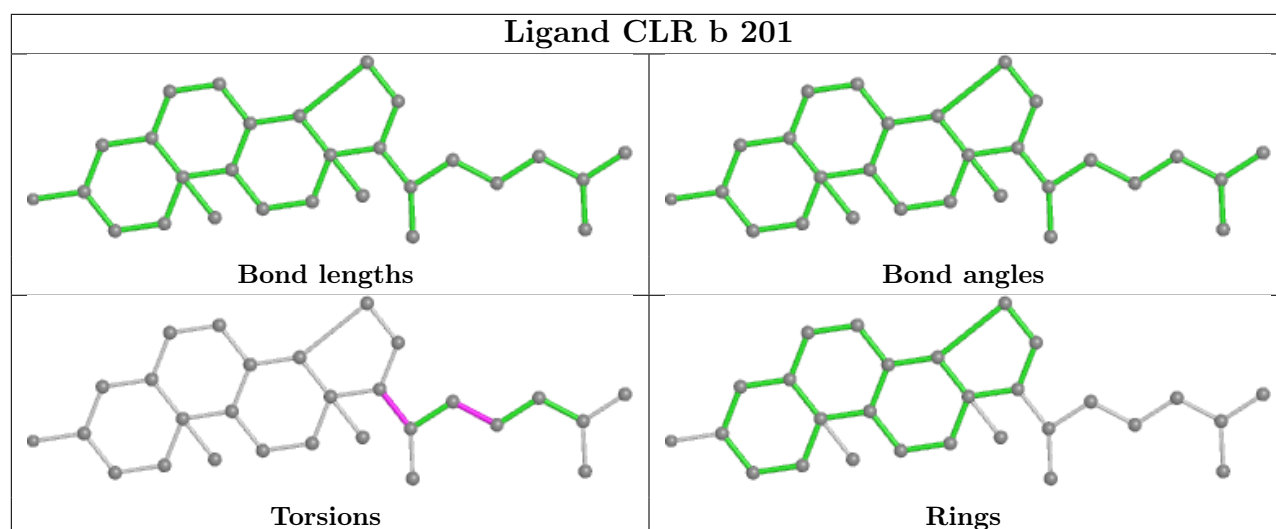
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	b	201	CLR	C20-C22-C23-C24
7	b	201	CLR	C16-C17-C20-C22
7	b	201	CLR	C13-C17-C20-C22
7	b	201	CLR	C13-C17-C20-C21

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.