wwPDB EM Validation Summary Report (i)

Jun 9, 2024 – 12:07 AM JST

PDB ID	:	8WXE
EMDB ID	:	EMD-37904
Title	:	Vgamma5Vdelta1 EH TCR-CD3 complex
Authors	:	Xin, W.; Huang, B.; Chi, X.; Xu, M.; Zhang, Y.; Li, X.; Su, Q.; Zhou, Q.
Deposited on	:	2023-10-28
Resolution	:	4.00 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 (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:

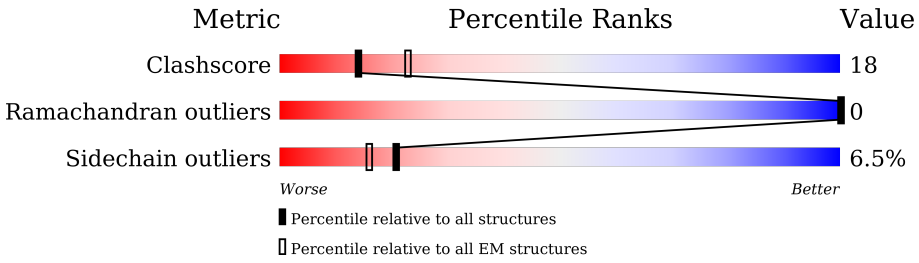
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.00 Å.

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



Metric	Whole archive (#Entries)	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	195	13% · 86%
1	b	195	14% · 86%
2	d	171	57% · 39%
3	e	207	49% · 49%
3	f	207	47% · 49%
4	g	182	55% · 43%
5	m	307	10% · 89%
6	n	331	11% · 89%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4388 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	28	Total	C	N	O	S	0	0
			226	157	33	35	1		
1	b	28	Total	C	N	O	S	0	0
			226	157	33	35	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

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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	106	Total	C	N	O	S	0	0
			853	550	133	162	8		
3	f	106	Total	C	N	O	S	0	0
			847	540	135	164	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	104	Total	C	N	O	S	0	0
			821	530	135	149	7		

- Molecule 5 is a protein called Signal peptide,flag tag,T cell receptor delta variable 1,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 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	115	ASP	-	linker	UNP A0A1B0GX56
m	116	PRO	-	linker	UNP A0A1B0GX56
m	117	GLY	-	linker	UNP A0A1B0GX56
m	118	GLY	-	linker	UNP A0A1B0GX56
m	119	LEU	-	linker	UNP A0A1B0GX56
m	120	ASN	-	linker	UNP A0A1B0GX56
m	121	THR	-	linker	UNP A0A1B0GX56
m	122	ASP	-	linker	UNP A0A1B0GX56
m	123	LYS	-	linker	UNP A0A1B0GX56
m	124	LEU	-	linker	UNP A0A1B0GX56
m	125	ILE	-	linker	UNP A0A1B0GX56
m	126	PHE	-	linker	UNP A0A1B0GX56
m	127	GLY	-	linker	UNP A0A1B0GX56
m	128	LYS	-	linker	UNP A0A1B0GX56
m	129	GLY	-	linker	UNP A0A1B0GX56
m	130	THR	-	linker	UNP A0A1B0GX56
m	131	ARG	-	linker	UNP A0A1B0GX56
m	132	VAL	-	linker	UNP A0A1B0GX56
m	133	THR	-	linker	UNP A0A1B0GX56
m	134	VAL	-	linker	UNP A0A1B0GX56

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Chain	Residue	Modelled	Actual	Comment	Reference
m	135	GLU	-	linker	UNP A0A1B0GX56
m	136	PRO	-	linker	UNP A0A1B0GX56
m	137	ARG	-	linker	UNP A0A1B0GX56

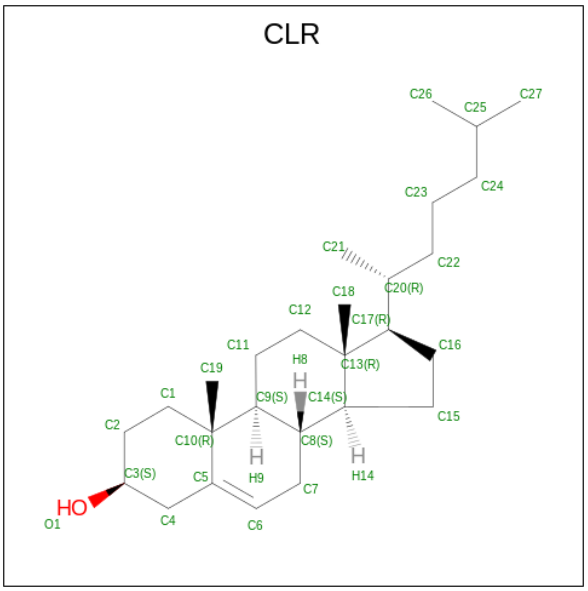
- Molecule 6 is a protein called Signal peptide,flag tag,T cell receptor gamma variable 5,T cell receptor gamma constant 1.

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

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	72	GLU	TYR	engineered mutation	UNP A0A0B4J1U4
n	86	HIS	ARG	engineered mutation	UNP A0A0B4J1U4
n	104	GLY	-	linker	UNP A0A0B4J1U4
n	105	ASN	-	linker	UNP A0A0B4J1U4
n	106	PRO	-	linker	UNP A0A0B4J1U4
n	107	LYS	-	linker	UNP A0A0B4J1U4
n	108	THR	-	linker	UNP A0A0B4J1U4
n	109	HIS	-	linker	UNP A0A0B4J1U4
n	110	TYR	-	linker	UNP A0A0B4J1U4
n	111	TYR	-	linker	UNP A0A0B4J1U4
n	112	LYS	-	linker	UNP A0A0B4J1U4
n	113	LYS	-	linker	UNP A0A0B4J1U4
n	114	LEU	-	linker	UNP A0A0B4J1U4
n	115	PHE	-	linker	UNP A0A0B4J1U4
n	116	GLY	-	linker	UNP A0A0B4J1U4
n	117	SER	-	linker	UNP A0A0B4J1U4
n	118	GLY	-	linker	UNP A0A0B4J1U4
n	119	THR	-	linker	UNP A0A0B4J1U4
n	120	THR	-	linker	UNP A0A0B4J1U4
n	121	LEU	-	linker	UNP A0A0B4J1U4
n	122	VAL	-	linker	UNP A0A0B4J1U4
n	123	VAL	-	linker	UNP A0A0B4J1U4
n	124	THR	-	linker	UNP A0A0B4J1U4

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



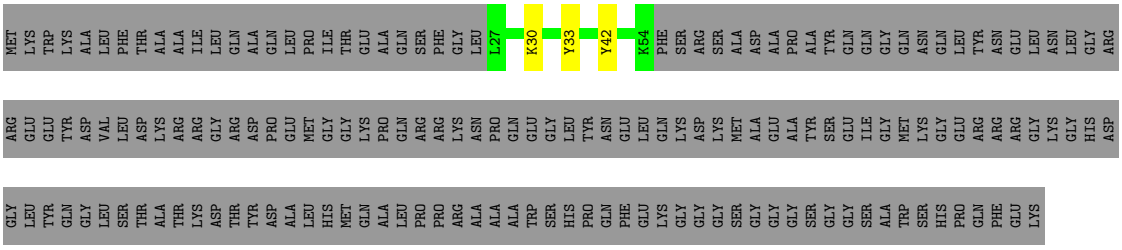
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	g	1	28	27	1	0

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.

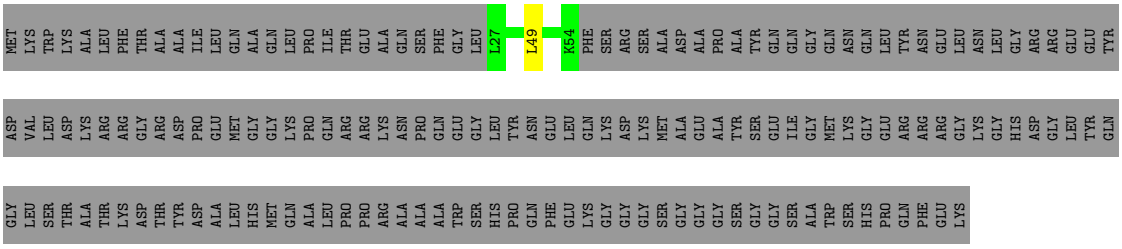
• Molecule 1: T-cell surface glycoprotein CD3 zeta chain

Chain a:



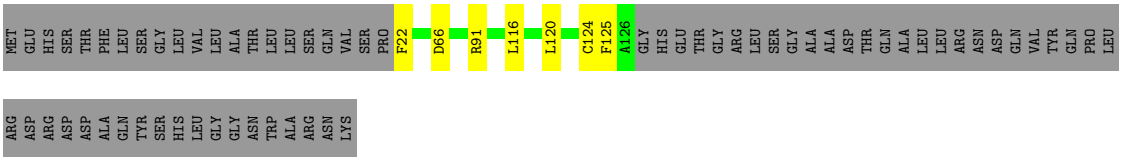
• Molecule 1: T-cell surface glycoprotein CD3 zeta chain

Chain b:



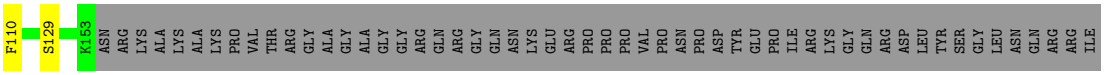
• Molecule 2: T-cell surface glycoprotein CD3 delta chain

Chain d:



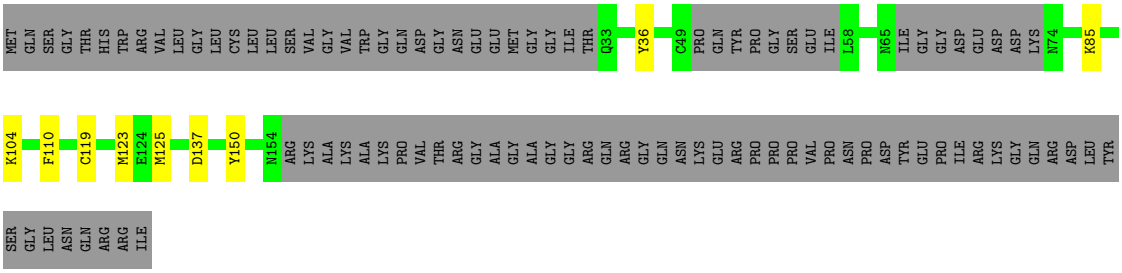
• Molecule 3: T-cell surface glycoprotein CD3 epsilon chain

Chain e:



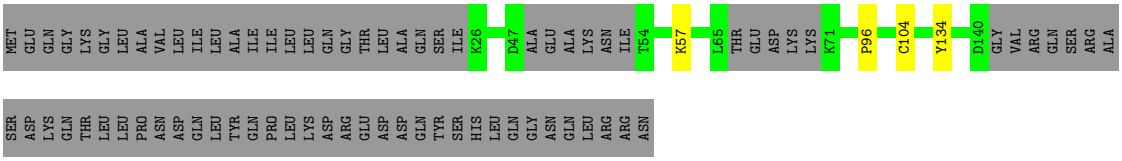
• Molecule 3: T-cell surface glycoprotein CD3 epsilon chain

Chain f:



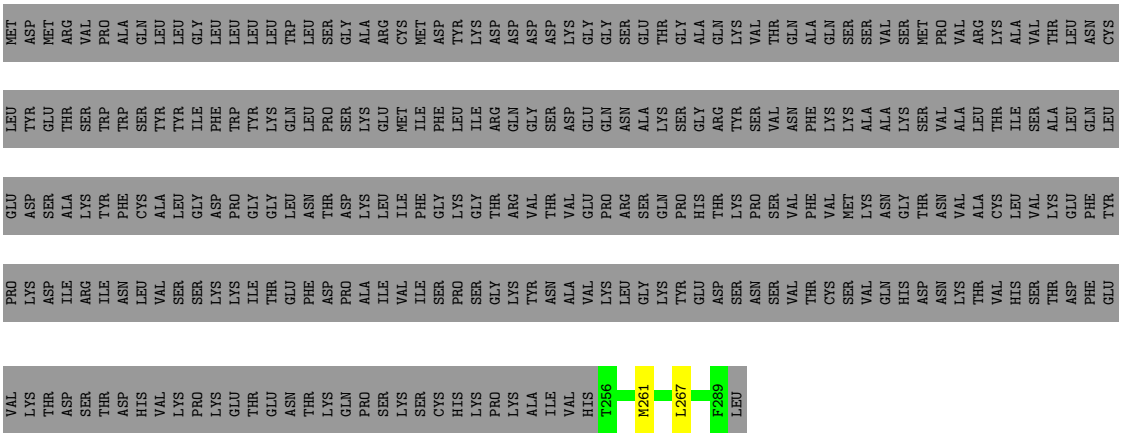
• Molecule 4: T-cell surface glycoprotein CD3 gamma chain

Chain g:



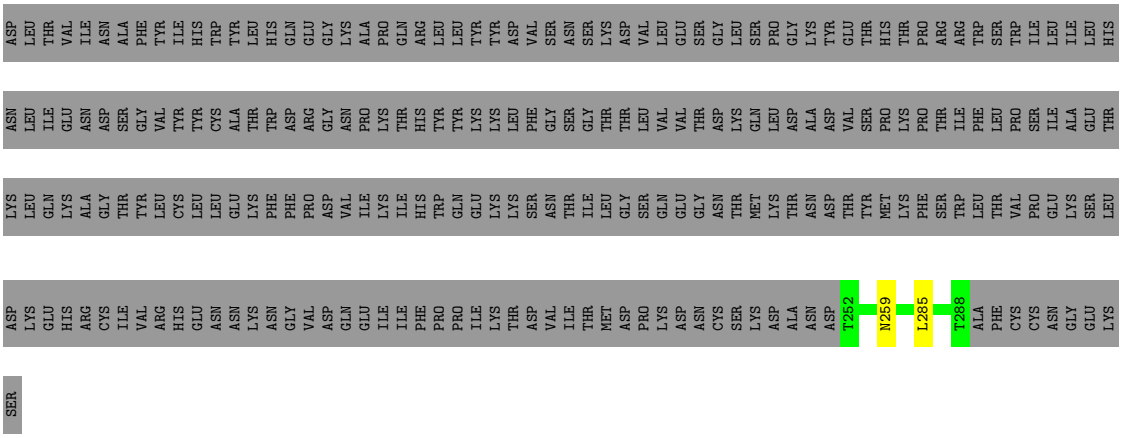
• Molecule 5: Signal peptide,flag tag,T cell receptor delta variable 1,T cell receptor delta constant

Chain m:



• Molecule 6: Signal peptide,flag tag,T cell receptor gamma variable 5,T cell receptor gamma constant 1

Chain n:


ASP LEU THR VAL ILE ASN ALA PHE TYR ILE HIS TRP TYR LEU HIS GLN GLU GLY LYS ALA PRO GLN ARG LEU LEU TYR TYR ASP VAL SER ASN SER LYS ASP VAL LEU GLU SER GLY LEU SER PRO GLY LYS TYR GLU THR HIS THR PRO ARG ARG TRP SER TRP ILE LEU ILE LEU HIS
ASN LEU ILE GLU ASN ASP SER GLY VAL TYR TYR CYS ALA THR TRP ASP ARG GLY ASN PRO LYS THR HIS TYR TYR LYS LYS LEU PHE GLY SER GLY THR THR LEU VAL VAL THR ASP LYS GLN LEU ASP ALA ASP VAL SER PRO LYS PRO THR ILE PHE LEU PRO SER ILE ALA GLU THR
LYS LEU GLN LYS ALA GLY THR TYR LEU CYS LEU LEU GLU LYS PHE PHE PRO ASP VAL ILE LYS ILE HIS TRP GLN GLU LYS LYS SER ASN THR ILE LEU GLY SER GLN GLU GLY ASN THR MET LYS THR ASN ASP THR TYR MET LYS PHE SER TRP LEU THR VAL PRO GLU LYS SER LEU
ASP LYS GLU HIS ARG CYS ILE VAL ARG HIS GLU ASN ASN LYS ASN GLY VAL ASP GLN GLU ILE ILE PHE PRO PRO ILE LYS THR ASP VAL ILE THR MET ASP PRO LYS ASP ASN CYS SER LYS ASP ALA ASN ASP T252 N259 L285 T288 ALA PHE CYS CYS ASN GLY GLU LYS
SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	342095	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 ($e^-/Å^2$)	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	0.30	0/230	0.49	0/311
1	b	0.32	0/230	0.45	0/311
2	d	0.24	0/829	0.53	0/1127
3	e	0.28	0/871	0.58	0/1182
3	f	0.27	0/863	0.58	0/1169
4	g	0.28	0/837	0.65	1/1124 (0.1%)
5	m	0.28	0/271	0.59	0/363
6	n	0.27	0/306	0.57	0/416
All	All	0.27	0/4437	0.57	1/6003 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	g	96	PRO	CA-N-CD	-9.43	98.30	111.50

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	226	0	250	0	0
1	b	226	0	250	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	817	0	828	0	0
3	e	853	0	831	0	0
3	f	847	0	819	0	0
4	g	821	0	806	0	0
5	m	268	0	296	0	0
6	n	302	0	332	0	0
7	g	28	0	46	0	0
All	All	4388	0	4458	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 18.

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	26/195 (13%)	26 (100%)	0	0	100	100
1	b	26/195 (13%)	26 (100%)	0	0	100	100
2	d	103/171 (60%)	97 (94%)	6 (6%)	0	100	100
3	e	100/207 (48%)	96 (96%)	4 (4%)	0	100	100
3	f	100/207 (48%)	92 (92%)	8 (8%)	0	100	100
4	g	98/182 (54%)	86 (88%)	12 (12%)	0	100	100
5	m	32/307 (10%)	32 (100%)	0	0	100	100
6	n	35/331 (11%)	34 (97%)	1 (3%)	0	100	100
All	All	520/1795 (29%)	489 (94%)	31 (6%)	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	25/154 (16%)	22 (88%)	3 (12%)	5 23
1	b	25/154 (16%)	24 (96%)	1 (4%)	31 57
2	d	93/147 (63%)	86 (92%)	7 (8%)	13 41
3	e	98/177 (55%)	93 (95%)	5 (5%)	24 52
3	f	97/177 (55%)	88 (91%)	9 (9%)	9 32
4	g	88/155 (57%)	85 (97%)	3 (3%)	37 61
5	m	30/272 (11%)	28 (93%)	2 (7%)	16 44
6	n	35/299 (12%)	33 (94%)	2 (6%)	20 49
All	All	491/1535 (32%)	459 (94%)	32 (6%)	21 45

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	m	261	MET
5	m	267	LEU
3	e	85	LYS
3	e	58	LEU
6	n	259	ASN

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

Mol	Chain	Res	Type
3	f	60	GLN
4	g	86	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 monosaccharides 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	g	201	-	31,31,31	0.28	0	48,48,48	0.48	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	g	201	-	-	7/10/68/68	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	g	201	CLR	C13-C17-C20-C21
7	g	201	CLR	C13-C17-C20-C22
7	g	201	CLR	C16-C17-C20-C22
7	g	201	CLR	C16-C17-C20-C21

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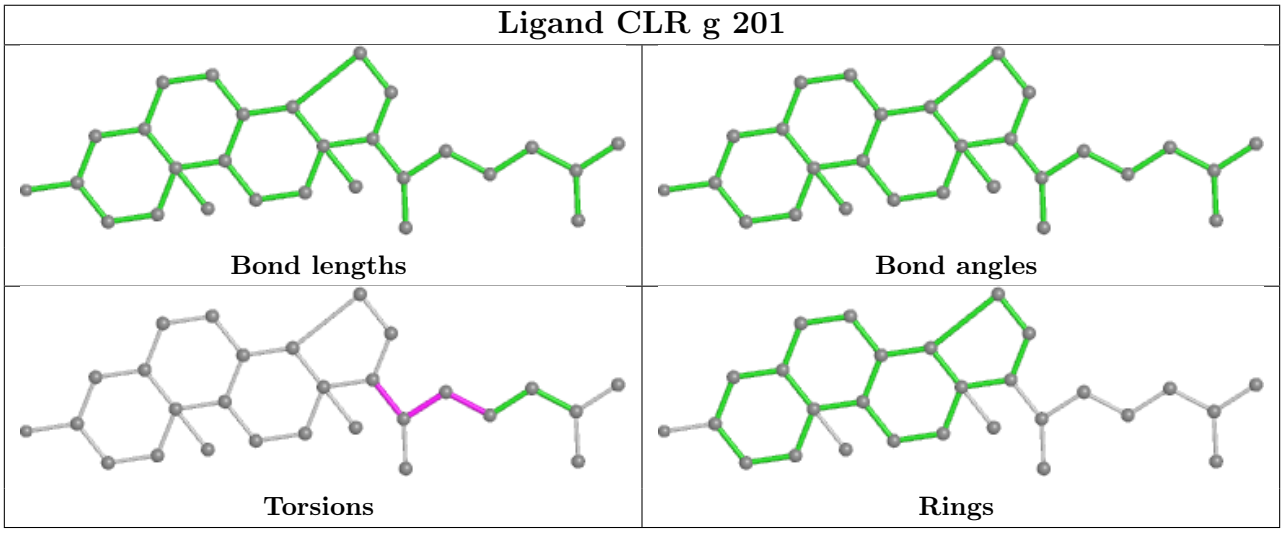
Mol	Chain	Res	Type	Atoms
7	g	201	CLR	C17-C20-C22-C23

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 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.



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.