



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:04 PM BST

PDB ID : 4UQK
EMDB ID: : EMD-2689
Title : Electron density map of GluA2em in complex with quisqualate and LY451646
Authors : Meyerson, J.R.; Kumar, J.; Chittori, S.; Rao, P.; Pierson, J.; Bartesaghi, A.; Mayer, M.L.; Subramaniam, S.
Deposited on : 2014-06-24
Resolution : 16.40 Å(reported)
Based on PDB ID : 1MM7

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

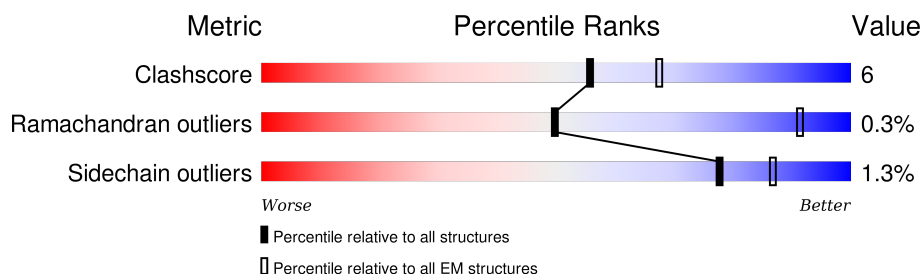
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 16.40 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	831	66% 10% 24%
1	B	831	66% 10% 24%
1	C	831	64% 12% • 24%
1	D	831	63% 12% • 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18784 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 GLUTAMATE RECEPTOR 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	631	Total	C	N	O	S	0	0
			4694	3001	759	911	23		
1	B	632	Total	C	N	O	S	0	0
			4699	3004	760	912	23		
1	C	632	Total	C	N	O	S	0	0
			4672	2984	758	908	22		
1	D	631	Total	C	N	O	S	0	0
			4667	2981	757	907	22		

There are 60 discrepancies between the modelled and reference sequences:

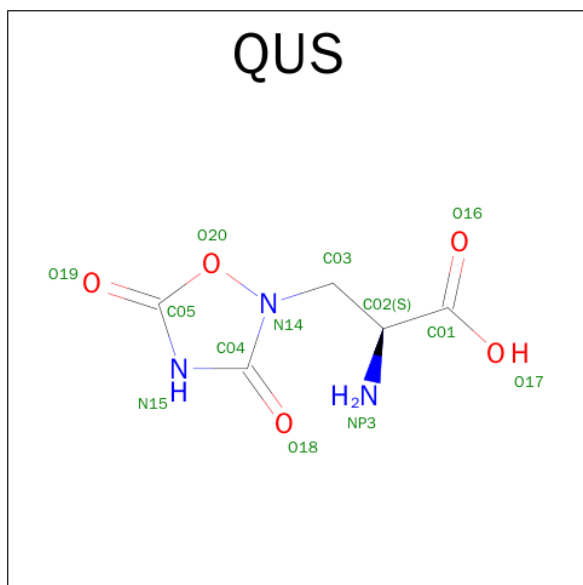
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	CONFLICT	UNP P19491
A	382	LEU	VAL	CONFLICT	UNP P19491
A	384	GLU	LEU	CONFLICT	UNP P19491
A	385	ASP	THR	CONFLICT	UNP P19491
A	589	ALA	CYS	CONFLICT	UNP P19491
A	631	THR	SER	CONFLICT	UNP P19491
A	744	ASN	THR	VARIANT	UNP P19491
A	745	ALA	PRO	VARIANT	UNP P19491
A	754	ASN	SER	VARIANT	UNP P19491
A	758	LEU	VAL	VARIANT	UNP P19491
A	827	GLY	-	EXPRESSION TAG	UNP P19491
A	828	LEU	-	EXPRESSION TAG	UNP P19491
A	829	VAL	-	EXPRESSION TAG	UNP P19491
A	830	PRO	-	EXPRESSION TAG	UNP P19491
A	831	ARG	-	EXPRESSION TAG	UNP P19491
B	241	GLU	ASN	CONFLICT	UNP P19491
B	382	LEU	VAL	CONFLICT	UNP P19491
B	384	GLU	LEU	CONFLICT	UNP P19491
B	385	ASP	THR	CONFLICT	UNP P19491
B	589	ALA	CYS	CONFLICT	UNP P19491
B	631	THR	SER	CONFLICT	UNP P19491
B	744	ASN	THR	VARIANT	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	745	ALA	PRO	VARIANT	UNP P19491
B	754	ASN	SER	VARIANT	UNP P19491
B	758	LEU	VAL	VARIANT	UNP P19491
B	827	GLY	-	EXPRESSION TAG	UNP P19491
B	828	LEU	-	EXPRESSION TAG	UNP P19491
B	829	VAL	-	EXPRESSION TAG	UNP P19491
B	830	PRO	-	EXPRESSION TAG	UNP P19491
B	831	ARG	-	EXPRESSION TAG	UNP P19491
C	241	GLU	ASN	CONFLICT	UNP P19491
C	382	LEU	VAL	CONFLICT	UNP P19491
C	384	GLU	LEU	CONFLICT	UNP P19491
C	385	ASP	THR	CONFLICT	UNP P19491
C	589	ALA	CYS	CONFLICT	UNP P19491
C	631	THR	SER	CONFLICT	UNP P19491
C	744	ASN	THR	VARIANT	UNP P19491
C	745	ALA	PRO	VARIANT	UNP P19491
C	754	ASN	SER	VARIANT	UNP P19491
C	758	LEU	VAL	VARIANT	UNP P19491
C	827	GLY	-	EXPRESSION TAG	UNP P19491
C	828	LEU	-	EXPRESSION TAG	UNP P19491
C	829	VAL	-	EXPRESSION TAG	UNP P19491
C	830	PRO	-	EXPRESSION TAG	UNP P19491
C	831	ARG	-	EXPRESSION TAG	UNP P19491
D	241	GLU	ASN	CONFLICT	UNP P19491
D	382	LEU	VAL	CONFLICT	UNP P19491
D	384	GLU	LEU	CONFLICT	UNP P19491
D	385	ASP	THR	CONFLICT	UNP P19491
D	589	ALA	CYS	CONFLICT	UNP P19491
D	631	THR	SER	CONFLICT	UNP P19491
D	744	ASN	THR	VARIANT	UNP P19491
D	745	ALA	PRO	VARIANT	UNP P19491
D	754	ASN	SER	VARIANT	UNP P19491
D	758	LEU	VAL	VARIANT	UNP P19491
D	827	GLY	-	EXPRESSION TAG	UNP P19491
D	828	LEU	-	EXPRESSION TAG	UNP P19491
D	829	VAL	-	EXPRESSION TAG	UNP P19491
D	830	PRO	-	EXPRESSION TAG	UNP P19491
D	831	ARG	-	EXPRESSION TAG	UNP P19491

- Molecule 2 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula: C₅H₇N₃O₅).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			13	5	3	5	
2	B	1	Total	C	N	O	0
			13	5	3	5	
2	C	1	Total	C	N	O	0
			13	5	3	5	
2	D	1	Total	C	N	O	0
			13	5	3	5	

SER	GLY	SER	SER	LYS	GLU	LYS	THR	SER	ALA	SER	LEU	SER	LEU	SER	ASN	VAL	ALA	GLY	VAL	PHE	TYR	ILE	LEU	VAL	GLY	LEU	GLY	LEU	GLY	LEU	ALA	LEU	ILE	GLU	PHE	CYS	TYR	LYS	SER	ARG	ALA	GLU	ALA	LYS	ARG	MET	LYS	GLY	LEU	VAL	PRO	ARG
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• Molecule 1: GLUTAMATE RECEPTOR 2

Chain C:

64%

12%

24%

ALA	LEU	ILE	GLU	PHE	CYS	TYR	LYS	SER	ARG	ALA	GLU	ALA	LYS	ARG	MET	LYS	GLY	LEU	VAL	PRO	ARG	SER	LEU	ALA	TYR	ILE	TRP	MET	CYS	ILE	ASP	VAL	PHE	ALA	TYR	GLU	ILE	TRP	GLU	ALA	LEU	PRO	SER	VAL		
6648			4685	7681	8692		5696		7700	7708		7711	8715	7718		7762	8772	8773																												
LEU	ILE	GLU	PHE	CYS	TYR	LYS	SER	ARG	ALA	GLU	ALA	LYS	ARG	MET	LYS	GLY	LEU	VAL	PRO	ARG	SER	LEU	ALA	TYR	ILE	TRP	MET	CYS	ILE	ASP	VAL	PHE	ALA	TYR	GLU	ILE	TRP	GLU	ALA	LEU	PRO	SER	VAL			
V165	K172	R191	D195	V205	V208	I209	H214	A223	P227	L232	L233	K234	I235	Q236	V242	S243	G244	F258	I259	E260	R261	L265	P271	T285	Y286	D287	Q290	V291	L299	P322	Q325	I329	V338	I360	W374	S375	E376									
V377	M380	D385	GLU	PRO	SER	GLY	ASN	ASP	THR	SER	GLY	LEU	ASN	K393	P404	M411	H412	L415	E419	H435	R453	D454	A455	K458	A477	P478	L483	E487	L498	R506	PRO	GLN	LYS	SER	LYS	PRO	GLY	PHE	ASN	TRP	LEU	ASP				
PRO	LEU	ALA	TYR	GLU	ILE	TRP	MET	CYS	ILE	ASP	VAL	PHE	ALA	TYR	ILE	GLY	VAL	ARG	PHE	SER	PRO	TYR	GLU	TRP	HIS	THR	GLU	GLU	GLN	SER	GLU	THR	ASN	GLY	PHE	ILE	ASN	TRP	LEU	ASP	VAL					
SER	LEU	ALA	PHE	MET	GLN	GLN	GLY	ALA	ASP	ILE	PRO	ARG	GLY	ILE	VAL	GLY	TRP	TRP	PHE	THR	ILE	ILE	THR	SER	SER	TYR	ALA	ASN	LEU	ALA	PHE	LEU	THR	VAL	TYR	ILE	LEU	MET	THR	GLY	LEU	VAL				
G648	A665	V681	H692	S696	Y700	H708	Y711	R715	C718	K752	E772	C773	ALA	LYS	ASP	GLY	LYS	GLY	THR	LEU	ILE	LYS	THR	SER	LEU	ASN	VAL	ALA	ALA	PHE	LEU	THR	VAL	PHE	TYR	ILE	LEU	VAL	GLY	LEU	LEU	ALA	MET	VAL		
ALA	LEU	ILE	GLU	PHE	CYS	TYR	LYS	SER	ARG	ALA	GLU	ALA	LYS	ARG	MET	LYS	GLY	LEU	VAL	PRO	ARG	SER	LEU	ALA	TYR	ILE	TRP	MET	CYS	ILE	ASP	VAL	PHE	ALA	TYR	GLU	ILE	TRP	GLU	ALA	LEU	PRO	SER	VAL		
VAL	SER	N10	A22	D23	Q24	E25	F29	M33	L43	T44	P45	M49	L50	F56	A57	A61	F62	F74	Y77	K80	F88	L92	H93	F96	I97	T98	P99	I111	Q112	M113	L117	A120	L124	I125	W130	Y135	L136	Y137	E376							

• Molecule 1: GLUTAMATE RECEPTOR 2

Chain D:

63%

12%

24%

LEU	GLY	ILE	PHE	Q642	ASP	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.36	0/4790	0.51	1/6520 (0.0%)
1	B	0.36	0/4795	0.51	1/6527 (0.0%)
1	C	0.34	1/4767 (0.0%)	0.50	1/6489 (0.0%)
1	D	0.34	1/4762 (0.0%)	0.50	1/6482 (0.0%)
All	All	0.35	2/19114 (0.0%)	0.50	4/26018 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	419	GLU	CB-CG	-5.41	1.41	1.52
1	C	419	GLU	CB-CG	-5.40	1.41	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	498	LEU	CA-CB-CG	5.52	128.00	115.30
1	D	498	LEU	CA-CB-CG	5.03	126.86	115.30
1	C	498	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4694	0	4378	55	0
1	B	4699	0	4380	51	0
1	C	4672	0	4346	61	0
1	D	4667	0	4344	66	0
2	A	13	0	6	0	0
2	B	13	0	6	0	0
2	C	13	0	6	0	0
2	D	13	0	6	0	0
All	All	18784	0	17472	229	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.

The worst 5 of 229 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:C:453:ARG:HH12	1:C:455:ALA:HA	1.39	0.87
1:D:453:ARG:HH12	1:D:455:ALA:HA	1.39	0.85
1:C:711:TYR:CZ	1:C:715:ARG:HD2	2.28	0.68
1:D:711:TYR:CZ	1:D:715:ARG:HD2	2.28	0.68
1:A:50:LEU:HD23	1:A:57:ALA:HB1	1.83	0.61

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	625/831 (75%)	594 (95%)	29 (5%)	2 (0%)	46 83
1	B	626/831 (75%)	596 (95%)	28 (4%)	2 (0%)	46 83
1	C	626/831 (75%)	592 (95%)	32 (5%)	2 (0%)	46 83
1	D	625/831 (75%)	590 (94%)	33 (5%)	2 (0%)	46 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2502/3324 (75%)	2372 (95%)	122 (5%)	8 (0%)	50 83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	LYS
1	A	456	ASP
1	B	172	LYS
1	B	456	ASP
1	C	172	LYS

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	470/708 (66%)	466 (99%)	4 (1%)	84 93
1	B	470/708 (66%)	466 (99%)	4 (1%)	84 93
1	C	467/708 (66%)	459 (98%)	8 (2%)	68 87
1	D	467/708 (66%)	459 (98%)	8 (2%)	68 87
All	All	1874/2832 (66%)	1850 (99%)	24 (1%)	78 89

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	404	PRO
1	C	498	LEU
1	D	642	GLN
1	C	411	ASN
1	C	453	ARG

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

Mol	Chain	Res	Type
1	A	83	ASN
1	A	435	HIS
1	B	435	HIS
1	D	83	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	QUS	A	1803	-	4,13,13	1.16	0	0,18,18	0.00	-
2	QUS	B	1803	-	4,13,13	1.12	0	0,18,18	0.00	-
2	QUS	C	1803	-	4,13,13	1.20	1 (25%)	0,18,18	0.00	-
2	QUS	D	1803	-	4,13,13	1.18	1 (25%)	0,18,18	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	QUS	A	1803	-	-	0/2/8/8	0/0/1/1
2	QUS	B	1803	-	-	0/2/8/8	0/0/1/1
2	QUS	C	1803	-	-	0/2/8/8	0/0/1/1
2	QUS	D	1803	-	-	0/2/8/8	0/0/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1803	QUS	C04-N15	2.12	1.36	1.34
2	C	1803	QUS	C04-N15	2.16	1.36	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.