



## 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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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

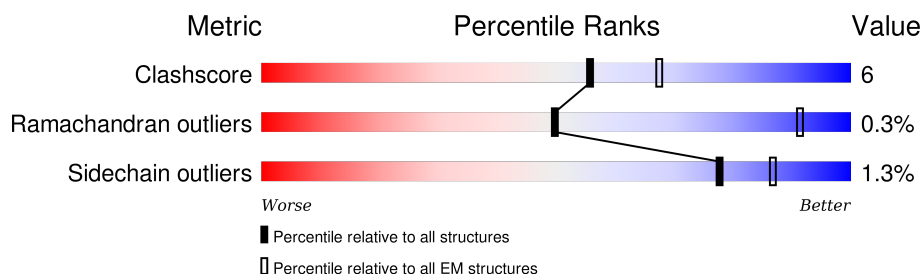
# 1 Overall quality at a glance

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  $\geq 3$ , 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:

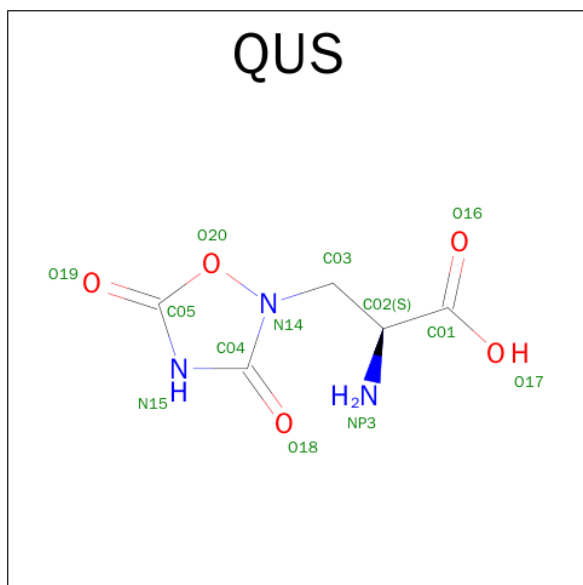
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	CONFLICT	UNP P19491
A	382	LEU	VAL	CONFLICT	UNP P19491
A	384	GLU	LEU	CONFLICT	UNP P19491
A	385	ASP	THR	CONFLICT	UNP P19491
A	589	ALA	CYS	CONFLICT	UNP P19491
A	631	THR	SER	CONFLICT	UNP P19491
A	744	ASN	THR	VARIANT	UNP P19491
A	745	ALA	PRO	VARIANT	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: C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O<sub>5</sub>).



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	PRO	TYR	GLU	LEU	ILE	GLY	VAL	TRP	THR	LEU	GLY	VAL	THR	GLY	GLY	LEU	LEU	ALA	MET	LEU	VAL													
6648			4685		7681		8692		5696		7700		8708		7711		8715		7718		8752		8772		7773		GLY	ALA	LYS	ASP	GLY	SER	LEU	ILE	ILE	THR	SER	ALA	TYR	GLU	ASP	ASN	VAL	ALA	THR											
SER	LEU	GLY	ALA	PHE	MET	GLN	GLN	GLY	ALA	ASP	ILE	SER	PRO	ARG	SER	LEU	GLY	GLY	ARG	ILE	VAL	ILE	VAL	PHE	GLY	LEU	VAL	ILE	SER	VAL	TRP	THR	PHE	THR	THR	GLU	GLU	THR	ASN	ALA	ALA	ALA	PHE	LEU	THR											
PRO	LEU	ALA	TYR	GLU	ILE	TRP	MET	CYS	ILE	VAL	PHE	ALA	ALA	TYR	ILE	VAL	VAL	SER	VAL	VAL	LEU	PHE	ARG	PRO	TYR	GLU	TRP	HIS	THR	GLU	GLU	THR	GLN	SER	SER	GLU	PRO	THR	ASN	GLY	GLY	GLN	VAL	ASN	THR											
V377			K380		D385	GLU	PRO	SER	SER	GLY	ASN	ASP	THR	SER	GLY	P404	H411	H412	L415		E419		H435		T438	GLY	TRP	HIS	THR	GLU	GLU	PHE	GLU	GLU	ASP	P478	L483	E487		L498		R506	PRO	GLN	LYS											
V165			K172		R191	D195	V205		V208	I209		E214		A223		F227		Q236	V242		S243		G244		F258	I259	E260	R261		L265		P271		T285		Y286	D287	Q290	V291		L299		P322		Q325		I329	V338		I360		W374		S375		E376
VAL	SER	N10	A22	D23	Q24	E25	F29		M33		L43	T44	P45	N49	L50	F56	A57	Q236	A61	F62		F74		Y77		K80		F88		L92	H93		F96	I97	T98	P99		I111	Q112	M113		L117		A120		L124	I125		W130		Y135	L136	Y137			

• 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	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	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.

All (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
1:B:50:LEU:HD23	1:B:57:ALA:HB1	1.82	0.61
1:C:50:LEU:HD23	1:C:57:ALA:HB1	1.82	0.61
1:D:50:LEU:HD23	1:D:57:ALA:HB1	1.83	0.59
1:D:235:ILE:HD13	1:D:242:VAL:HG21	1.85	0.59
1:B:10:ASN:N	1:B:10:ASN:HD22	2.01	0.58
1:A:235:ILE:HD13	1:A:242:VAL:HG21	1.85	0.58
1:A:10:ASN:N	1:A:10:ASN:HD22	2.01	0.58
1:C:10:ASN:HD22	1:C:10:ASN:N	2.01	0.58
1:B:235:ILE:HD13	1:B:242:VAL:HG21	1.85	0.58
1:B:93:HIS:ND1	1:B:322:PRO:HB3	2.19	0.57
1:C:99:PRO:HA	1:C:113:MET:HB2	1.87	0.57
1:B:99:PRO:HA	1:B:113:MET:HB2	1.87	0.56
1:A:99:PRO:HA	1:A:113:MET:HB2	1.87	0.56
1:C:235:ILE:HD13	1:C:242:VAL:HG21	1.85	0.56
1:C:93:HIS:ND1	1:C:322:PRO:HB3	2.19	0.56
1:B:77:TYR:CE2	1:B:98:THR:HG21	2.40	0.56
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.41	0.56
1:A:376:GLU:HG3	1:A:377:VAL:HG13	1.88	0.56
1:D:10:ASN:N	1:D:10:ASN:HD22	2.01	0.56
1:C:227:PHE:CD1	1:C:244:GLY:HA3	2.41	0.56
1:B:209:ILE:HA	1:B:214:HIS:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HA	1:A:214:HIS:CD2	2.41	0.56
1:D:299:LEU:HD11	1:D:332:ALA:HB2	1.88	0.56
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.41	0.56
1:C:209:ILE:HA	1:C:214:HIS:CD2	2.41	0.55
1:C:376:GLU:HG3	1:C:377:VAL:HG13	1.88	0.55
1:D:227:PHE:CD1	1:D:244:GLY:HA3	2.41	0.55
1:D:99:PRO:HA	1:D:113:MET:HB2	1.87	0.55
1:C:77:TYR:CE2	1:C:98:THR:HG21	2.41	0.55
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.41	0.55
1:D:77:TYR:CE2	1:D:98:THR:HG21	2.41	0.55
1:B:376:GLU:HG3	1:B:377:VAL:HG13	1.88	0.55
1:A:299:LEU:HD11	1:A:332:ALA:HB2	1.88	0.55
1:A:77:TYR:CE2	1:A:98:THR:HG21	2.41	0.55
1:A:62:PHE:HE2	1:A:92:LEU:HD12	1.73	0.54
1:D:376:GLU:HG3	1:D:377:VAL:HG13	1.88	0.54
1:D:62:PHE:HE2	1:D:92:LEU:HD12	1.72	0.54
1:D:453:ARG:NH1	1:D:454:ASP:O	2.40	0.54
1:C:453:ARG:NH1	1:C:454:ASP:O	2.40	0.53
1:D:453:ARG:HH12	1:D:455:ALA:CA	2.18	0.53
1:C:62:PHE:HE2	1:C:92:LEU:HD12	1.73	0.53
1:B:62:PHE:HE2	1:B:92:LEU:HD12	1.73	0.53
1:A:205:VAL:O	1:A:209:ILE:HG13	2.10	0.52
1:B:205:VAL:O	1:B:209:ILE:HG13	2.10	0.52
1:D:205:VAL:O	1:D:209:ILE:HG13	2.10	0.51
1:C:205:VAL:O	1:C:209:ILE:HG13	2.10	0.51
1:B:756:GLN:HA	1:B:756:GLN:OE1	2.10	0.51
1:C:642:GLN:OE1	1:C:644:GLU:N	2.44	0.51
1:D:642:GLN:OE1	1:D:644:GLU:N	2.44	0.51
1:A:74:PHE:CZ	1:A:285:THR:HG23	2.46	0.51
1:D:74:PHE:CZ	1:D:285:THR:HG23	2.46	0.50
1:C:453:ARG:HD2	1:C:458:LYS:HA	1.94	0.50
1:A:756:GLN:HA	1:A:756:GLN:OE1	2.10	0.50
1:B:74:PHE:CZ	1:B:285:THR:HG23	2.47	0.50
1:D:43:LEU:O	1:D:45:PRO:HD3	2.11	0.50
1:D:453:ARG:HD2	1:D:458:LYS:HA	1.94	0.49
1:B:43:LEU:O	1:B:45:PRO:HD3	2.12	0.49
1:D:50:LEU:HD22	1:D:61:ALA:HB2	1.95	0.49
1:A:83:ASN:ND2	1:B:80:LYS:HA	2.27	0.49
1:C:50:LEU:HD22	1:C:61:ALA:HB2	1.95	0.49
1:B:431:GLU:HG3	1:B:758:LEU:HD21	1.95	0.49
1:C:56:PHE:CE2	1:D:91:THR:HG21	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LEU:O	1:C:45:PRO:HD3	2.12	0.49
1:C:74:PHE:CZ	1:C:285:THR:HG23	2.47	0.49
1:C:646:ALA:O	1:C:700:TYR:HA	2.13	0.49
1:C:80:LYS:HA	1:D:83:ASN:ND2	2.27	0.49
1:A:43:LEU:O	1:A:45:PRO:HD3	2.11	0.49
1:D:646:ALA:O	1:D:700:TYR:HA	2.13	0.49
1:A:91:THR:HG21	1:B:56:PHE:CE2	2.47	0.48
1:A:431:GLU:HG3	1:A:758:LEU:HD21	1.95	0.48
1:A:50:LEU:HD22	1:A:61:ALA:HB2	1.95	0.48
1:B:50:LEU:HD22	1:B:61:ALA:HB2	1.95	0.48
1:A:258:PHE:HD2	1:A:259:ILE:HD12	1.79	0.48
1:C:258:PHE:HD2	1:C:259:ILE:HD12	1.79	0.48
1:D:29:PHE:O	1:D:33:MET:HG2	2.14	0.47
1:D:97:ILE:HG13	1:D:111:ILE:HB	1.96	0.47
1:C:195:ASP:HA	1:C:223:ALA:HB3	1.96	0.47
1:B:124:LEU:HD13	1:B:380:MET:HE1	1.96	0.47
1:B:195:ASP:HA	1:B:223:ALA:HB3	1.96	0.47
1:D:258:PHE:HD2	1:D:259:ILE:HD12	1.79	0.47
1:C:124:LEU:HD13	1:C:380:MET:HE1	1.96	0.47
1:A:208:VAL:HG12	1:A:214:HIS:HB3	1.97	0.47
1:B:97:ILE:HG13	1:B:111:ILE:HB	1.97	0.47
1:D:648:GLY:HA3	1:D:681:VAL:O	2.15	0.47
1:D:195:ASP:HA	1:D:223:ALA:HB3	1.96	0.47
1:B:135:TYR:CE2	1:B:137:TYR:HB3	2.50	0.47
1:A:29:PHE:O	1:A:33:MET:HG2	2.14	0.46
1:D:62:PHE:CE2	1:D:92:LEU:HD12	2.51	0.46
1:D:642:GLN:NE2	1:D:645:ILE:HD12	2.30	0.46
1:B:29:PHE:O	1:B:33:MET:HG2	2.15	0.46
1:A:97:ILE:HG13	1:A:111:ILE:HB	1.97	0.46
1:A:195:ASP:HA	1:A:223:ALA:HB3	1.96	0.46
1:A:135:TYR:CE2	1:A:137:TYR:HB3	2.50	0.46
1:B:258:PHE:HD2	1:B:259:ILE:HD12	1.79	0.46
1:D:22:ALA:HB1	1:D:25:GLU:HB2	1.97	0.46
1:C:483:LEU:O	1:C:487:GLU:HG3	2.16	0.46
1:D:135:TYR:CE2	1:D:137:TYR:HB3	2.50	0.46
1:C:135:TYR:CE2	1:C:137:TYR:HB3	2.50	0.46
1:C:208:VAL:HG12	1:C:214:HIS:HB3	1.97	0.46
1:C:29:PHE:O	1:C:33:MET:HG2	2.15	0.46
1:D:23:ASP:HB3	1:D:271:PRO:HB2	1.98	0.46
1:D:483:LEU:O	1:D:487:GLU:HG3	2.16	0.46
1:C:209:ILE:CD1	1:C:234:LYS:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HD12	1:A:120:ALA:HB3	1.98	0.45
1:B:208:VAL:HG12	1:B:214:HIS:HB3	1.97	0.45
1:C:62:PHE:CE2	1:C:92:LEU:HD12	2.51	0.45
1:B:22:ALA:HB1	1:B:25:GLU:HB2	1.98	0.45
1:C:97:ILE:HG13	1:C:111:ILE:HB	1.97	0.45
1:B:209:ILE:CD1	1:B:234:LYS:HB2	2.46	0.45
1:C:642:GLN:NE2	1:C:645:ILE:HD12	2.30	0.45
1:C:648:GLY:HA3	1:C:681:VAL:O	2.15	0.45
1:B:62:PHE:CE2	1:B:92:LEU:HD12	2.51	0.45
1:C:22:ALA:HB1	1:C:25:GLU:HB2	1.98	0.45
1:B:117:LEU:HD12	1:B:120:ALA:HB3	1.98	0.45
1:D:208:VAL:HG12	1:D:214:HIS:HB3	1.97	0.45
1:A:23:ASP:HB3	1:A:271:PRO:HB2	1.98	0.45
1:A:62:PHE:CE2	1:A:88:PHE:HB3	2.52	0.45
1:C:117:LEU:HD12	1:C:120:ALA:HB3	1.98	0.45
1:A:22:ALA:HB1	1:A:25:GLU:HB2	1.97	0.45
1:C:453:ARG:HH12	1:C:455:ALA:CA	2.18	0.45
1:A:209:ILE:CD1	1:A:234:LYS:HB2	2.47	0.45
1:C:23:ASP:HB3	1:C:271:PRO:HB2	1.98	0.45
1:A:165:VAL:HG22	1:A:165:VAL:O	2.17	0.45
1:A:98:THR:HA	1:A:99:PRO:HD3	1.80	0.45
1:B:23:ASP:HB3	1:B:271:PRO:HB2	1.98	0.44
1:D:261:ARG:O	1:D:265:LEU:HG	2.17	0.44
1:D:125:ILE:HG23	1:D:130:TRP:HB2	1.99	0.44
1:D:117:LEU:HD12	1:D:120:ALA:HB3	1.98	0.44
1:C:261:ARG:O	1:C:265:LEU:HG	2.17	0.44
1:A:125:ILE:HG23	1:A:130:TRP:HB2	1.99	0.44
1:B:96:PHE:CE2	1:B:98:THR:HB	2.53	0.44
1:A:130:TRP:CH2	1:A:191:ARG:HB3	2.53	0.44
1:A:261:ARG:O	1:A:265:LEU:HG	2.17	0.44
1:D:62:PHE:CE2	1:D:88:PHE:HB3	2.52	0.44
1:D:165:VAL:HG22	1:D:165:VAL:O	2.17	0.44
1:B:130:TRP:CE2	1:B:191:ARG:HD3	2.53	0.44
1:D:209:ILE:CD1	1:D:234:LYS:HB2	2.47	0.44
1:A:62:PHE:CE2	1:A:92:LEU:HD12	2.51	0.44
1:C:477:ALA:HB1	1:C:478:PRO:HD2	2.00	0.44
1:C:125:ILE:HG23	1:C:130:TRP:HB2	1.99	0.44
1:C:62:PHE:CE2	1:C:88:PHE:HB3	2.52	0.44
1:A:477:ALA:HB1	1:A:478:PRO:HD2	1.99	0.44
1:B:165:VAL:HG22	1:B:165:VAL:O	2.18	0.44
1:C:287:ASP:O	1:C:291:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ARG:O	1:B:265:LEU:HG	2.17	0.44
1:C:49:ASN:C	1:C:50:LEU:HD12	2.38	0.44
1:D:49:ASN:C	1:D:50:LEU:HD12	2.38	0.44
1:D:96:PHE:CE2	1:D:98:THR:HB	2.53	0.44
1:C:130:TRP:CH2	1:C:191:ARG:HB3	2.53	0.44
1:A:49:ASN:C	1:A:50:LEU:HD12	2.38	0.44
1:A:96:PHE:CE2	1:A:98:THR:HB	2.53	0.44
1:C:290:GLN:HG2	1:C:338:VAL:HG21	2.00	0.43
1:D:404:PRO:HB3	1:D:711:TYR:CE1	2.53	0.43
1:D:715:ARG:HA	1:D:772:GLU:HG2	2.01	0.43
1:C:96:PHE:CE2	1:C:98:THR:HB	2.53	0.43
1:B:130:TRP:CH2	1:B:191:ARG:HB3	2.53	0.43
1:A:287:ASP:O	1:A:291:VAL:HG23	2.18	0.43
1:B:62:PHE:CE2	1:B:88:PHE:HB3	2.52	0.43
1:D:130:TRP:CE2	1:D:191:ARG:HD3	2.54	0.43
1:B:477:ALA:HB1	1:B:478:PRO:HD2	1.99	0.43
1:C:718:CYS:CB	1:C:773:CYS:SG	3.06	0.43
1:C:404:PRO:HB3	1:C:711:TYR:CE1	2.53	0.43
1:B:125:ILE:HG23	1:B:130:TRP:HB2	1.99	0.43
1:D:287:ASP:O	1:D:291:VAL:HG23	2.18	0.43
1:C:130:TRP:CE2	1:C:191:ARG:HD3	2.53	0.43
1:D:718:CYS:CB	1:D:773:CYS:SG	3.06	0.43
1:B:287:ASP:O	1:B:291:VAL:HG23	2.18	0.43
1:B:209:ILE:HD11	1:B:235:ILE:HG23	2.01	0.43
1:B:290:GLN:HG2	1:B:338:VAL:HG21	2.00	0.43
1:C:165:VAL:O	1:C:165:VAL:HG22	2.18	0.43
1:C:97:ILE:N	1:C:97:ILE:HD12	2.34	0.43
1:D:130:TRP:CH2	1:D:191:ARG:HB3	2.53	0.43
1:B:49:ASN:C	1:B:50:LEU:HD12	2.38	0.43
1:B:360:ILE:HD11	1:B:374:TRP:HB2	2.01	0.43
1:C:715:ARG:HA	1:C:772:GLU:HG2	2.01	0.42
1:A:233:LEU:HD23	1:A:236:GLN:OE1	2.19	0.42
1:A:130:TRP:CE2	1:A:191:ARG:HD3	2.54	0.42
1:B:233:LEU:HD23	1:B:236:GLN:OE1	2.19	0.42
1:A:209:ILE:HD11	1:A:235:ILE:HG23	2.01	0.42
1:B:97:ILE:N	1:B:97:ILE:HD12	2.34	0.42
1:A:360:ILE:HD11	1:A:374:TRP:HB2	2.01	0.42
1:D:477:ALA:HB1	1:D:478:PRO:HD2	2.00	0.42
1:A:97:ILE:N	1:A:97:ILE:HD12	2.35	0.42
1:D:97:ILE:N	1:D:97:ILE:HD12	2.34	0.42
1:C:360:ILE:HD11	1:C:374:TRP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:LEU:HD23	1:D:236:GLN:OE1	2.19	0.42
1:D:235:ILE:HG13	1:D:235:ILE:H	1.73	0.42
1:C:209:ILE:HD11	1:C:235:ILE:HG23	2.01	0.41
1:C:233:LEU:HD23	1:C:236:GLN:OE1	2.19	0.41
1:C:232:LEU:O	1:C:236:GLN:HB2	2.20	0.41
1:C:435:HIS:CE1	1:C:752:LYS:HD3	2.55	0.41
1:D:360:ILE:HD11	1:D:374:TRP:HB2	2.01	0.41
1:A:232:LEU:O	1:A:236:GLN:HB2	2.20	0.41
1:D:435:HIS:CE1	1:D:752:LYS:HD3	2.55	0.41
1:D:114:ARG:HA	1:D:115:PRO:HD3	1.92	0.41
1:D:209:ILE:HD11	1:D:235:ILE:HG23	2.01	0.41
1:B:232:LEU:O	1:B:236:GLN:HB2	2.21	0.41
1:D:232:LEU:O	1:D:236:GLN:HB2	2.20	0.41
1:B:192:VAL:HB	1:B:220:TYR:CD1	2.56	0.41
1:A:192:VAL:HB	1:A:220:TYR:CD1	2.56	0.41
1:D:288:ALA:O	1:D:292:MET:HG3	2.21	0.41
1:B:480:THR:HG21	1:B:730:LYS:HD2	2.03	0.41
1:D:127:TYR:CE1	1:D:382:LEU:HD21	2.56	0.41
1:A:127:TYR:CE1	1:A:382:LEU:HD21	2.56	0.41
1:B:114:ARG:HA	1:B:115:PRO:HD3	1.92	0.41
1:B:763:LYS:O	1:B:767:TRP:HB2	2.21	0.41
1:C:412:HIS:HA	1:C:415:LEU:HD12	2.03	0.41
1:A:480:THR:HG21	1:A:730:LYS:HD2	2.03	0.41
1:D:192:VAL:HB	1:D:220:TYR:CD1	2.56	0.40
1:C:692:ARG:O	1:C:696:SER:HB3	2.21	0.40
1:C:325:GLN:O	1:C:329:ILE:HG13	2.22	0.40
1:D:692:ARG:O	1:D:696:SER:HB3	2.21	0.40
1:A:10:ASN:N	1:A:10:ASN:ND2	2.69	0.40
1:A:299:LEU:CD1	1:A:332:ALA:HB2	2.51	0.40
1:A:321:VAL:HA	1:A:322:PRO:HD3	1.86	0.40
1:D:299:LEU:CD1	1:D:332:ALA:HB2	2.51	0.40
1:A:288:ALA:O	1:A:292:MET:HG3	2.21	0.40
1:D:266:GLU:HG2	1:D:268:LYS:H	1.86	0.40
1:D:325:GLN:O	1:D:329:ILE:HG13	2.22	0.40
1:D:143:LEU:HD22	1:D:143:LEU:N	2.37	0.40
1:B:18:PHE:HA	1:B:19:PRO:HD3	1.96	0.40
1:A:375:SER:HB3	1:A:378:ASP:HB2	2.03	0.40
1:A:763:LYS:O	1:A:767:TRP:HB2	2.21	0.40
1:A:325:GLN:O	1:A:329:ILE:HG13	2.22	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 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
All	All	2502/3324 (75%)	2372 (95%)	122 (5%)	8 (0%)	50	83

All (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
1	D	172	LYS
1	D	665	ALA
1	C	665	ALA

### 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	470/708 (66%)	466 (99%)	4 (1%)	84	93
1	B	470/708 (66%)	466 (99%)	4 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	299	LEU
1	A	498	LEU
1	A	708	MET
1	B	10	ASN
1	B	299	LEU
1	B	498	LEU
1	B	708	MET
1	C	10	ASN
1	C	299	LEU
1	C	404	PRO
1	C	411	ASN
1	C	453	ARG
1	C	498	LEU
1	C	642	GLN
1	C	708	MET
1	D	10	ASN
1	D	299	LEU
1	D	404	PRO
1	D	411	ASN
1	D	453	ARG
1	D	498	LEU
1	D	642	GLN
1	D	708	MET

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.