



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 15, 2019 – 03:40 PM EDT

PDB ID : 6PVQ  
EMDB ID: : EMD-20497  
Title : Cryo-EM structure of mouse TRPV3-Y564A in intermediate state at 37 degrees Celsius  
Authors : Singh, A.K.; McGoldrick, L.L.; Sobolevsky, A.I.  
Deposited on : 2019-07-21  
Resolution : 4.75 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

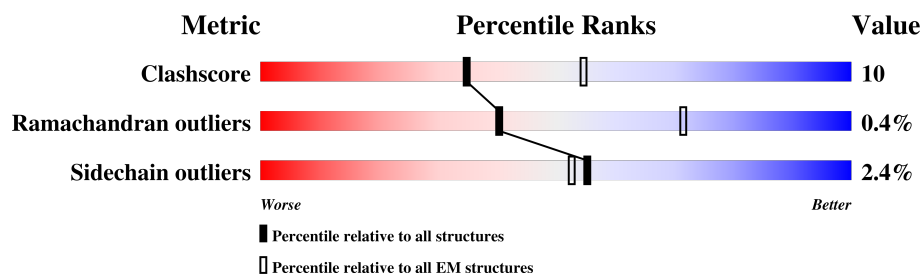
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.75 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	808	
1	B	808	
1	C	808	
1	D	808	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17640 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 Transient receptor potential cation channel subfamily V member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	562	Total	C	N	O	S	0	0
			4581	2938	781	837	25		
1	B	518	Total	C	N	O	S	0	0
			4239	2736	717	761	25		
1	C	562	Total	C	N	O	S	0	0
			4581	2938	781	837	25		
1	D	518	Total	C	N	O	S	0	0
			4239	2736	717	761	25		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	564	ALA	TYR	engineered mutation	UNP Q8K424
A	792	LEU	-	expression tag	UNP Q8K424
A	793	VAL	-	expression tag	UNP Q8K424
A	794	PRO	-	expression tag	UNP Q8K424
A	795	ARG	-	expression tag	UNP Q8K424
A	796	GLY	-	expression tag	UNP Q8K424
A	797	SER	-	expression tag	UNP Q8K424
A	798	ALA	-	expression tag	UNP Q8K424
A	799	ALA	-	expression tag	UNP Q8K424
A	800	ALA	-	expression tag	UNP Q8K424
A	801	TRP	-	expression tag	UNP Q8K424
A	802	SER	-	expression tag	UNP Q8K424
A	803	HIS	-	expression tag	UNP Q8K424
A	804	PRO	-	expression tag	UNP Q8K424
A	805	GLN	-	expression tag	UNP Q8K424
A	806	PHE	-	expression tag	UNP Q8K424
A	807	GLU	-	expression tag	UNP Q8K424
A	808	LYS	-	expression tag	UNP Q8K424
B	564	ALA	TYR	engineered mutation	UNP Q8K424
B	792	LEU	-	expression tag	UNP Q8K424
B	793	VAL	-	expression tag	UNP Q8K424

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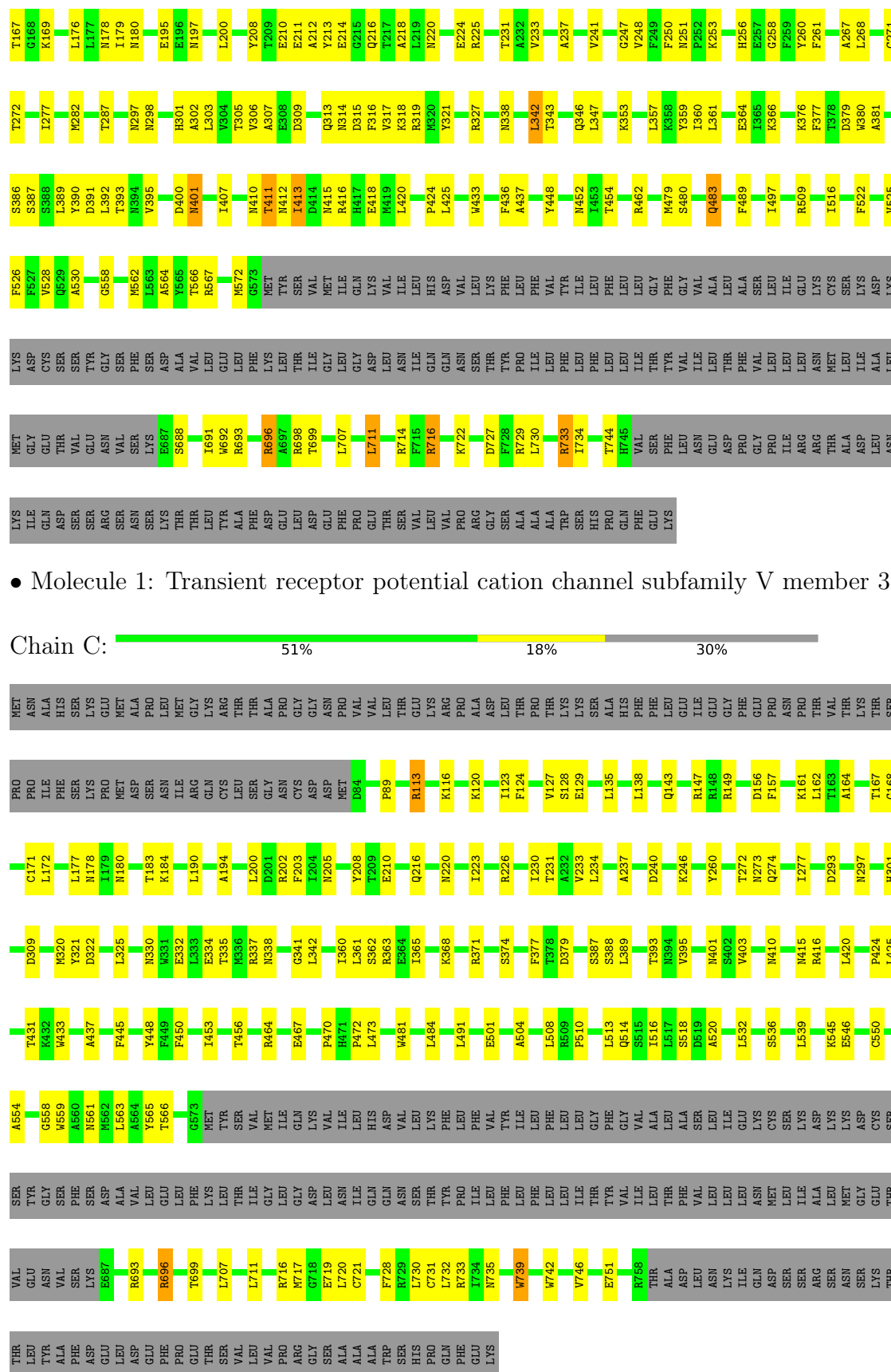
Chain	Residue	Modelled	Actual	Comment	Reference
B	794	PRO	-	expression tag	UNP Q8K424
B	795	ARG	-	expression tag	UNP Q8K424
B	796	GLY	-	expression tag	UNP Q8K424
B	797	SER	-	expression tag	UNP Q8K424
B	798	ALA	-	expression tag	UNP Q8K424
B	799	ALA	-	expression tag	UNP Q8K424
B	800	ALA	-	expression tag	UNP Q8K424
B	801	TRP	-	expression tag	UNP Q8K424
B	802	SER	-	expression tag	UNP Q8K424
B	803	HIS	-	expression tag	UNP Q8K424
B	804	PRO	-	expression tag	UNP Q8K424
B	805	GLN	-	expression tag	UNP Q8K424
B	806	PHE	-	expression tag	UNP Q8K424
B	807	GLU	-	expression tag	UNP Q8K424
B	808	LYS	-	expression tag	UNP Q8K424
C	564	ALA	TYR	engineered mutation	UNP Q8K424
C	792	LEU	-	expression tag	UNP Q8K424
C	793	VAL	-	expression tag	UNP Q8K424
C	794	PRO	-	expression tag	UNP Q8K424
C	795	ARG	-	expression tag	UNP Q8K424
C	796	GLY	-	expression tag	UNP Q8K424
C	797	SER	-	expression tag	UNP Q8K424
C	798	ALA	-	expression tag	UNP Q8K424
C	799	ALA	-	expression tag	UNP Q8K424
C	800	ALA	-	expression tag	UNP Q8K424
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C	802	SER	-	expression tag	UNP Q8K424
C	803	HIS	-	expression tag	UNP Q8K424
C	804	PRO	-	expression tag	UNP Q8K424
C	805	GLN	-	expression tag	UNP Q8K424
C	806	PHE	-	expression tag	UNP Q8K424
C	807	GLU	-	expression tag	UNP Q8K424
C	808	LYS	-	expression tag	UNP Q8K424
D	564	ALA	TYR	engineered mutation	UNP Q8K424
D	792	LEU	-	expression tag	UNP Q8K424
D	793	VAL	-	expression tag	UNP Q8K424
D	794	PRO	-	expression tag	UNP Q8K424
D	795	ARG	-	expression tag	UNP Q8K424
D	796	GLY	-	expression tag	UNP Q8K424
D	797	SER	-	expression tag	UNP Q8K424
D	798	ALA	-	expression tag	UNP Q8K424
D	799	ALA	-	expression tag	UNP Q8K424

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Chain	Residue	Modelled	Actual	Comment	Reference
D	800	ALA	-	expression tag	UNP Q8K424
D	801	TRP	-	expression tag	UNP Q8K424
D	802	SER	-	expression tag	UNP Q8K424
D	803	HIS	-	expression tag	UNP Q8K424
D	804	PRO	-	expression tag	UNP Q8K424
D	805	GLN	-	expression tag	UNP Q8K424
D	806	PHE	-	expression tag	UNP Q8K424
D	807	GLU	-	expression tag	UNP Q8K424
D	808	LYS	-	expression tag	UNP Q8K424





Chain D:  46% 17% . 36%

ARG	ARG	THR	ALA	ASP	LEU	ASN	LYS	ILE	GLY	GLN	ASP	SER	SER	ARG	THR	THR	ALA	PRO	GLY	GLY	LYS	PRO	MET	ALA	HIS	SER	LYS	GLU	LEU	ALA	ASP	ASN	LEU	PRO	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR	LYS	THR	THR
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	101814	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 ( $e^-/\text{\AA}^2$ )	57.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.43	0/4682	0.66	2/6339 (0.0%)
1	B	0.42	0/4332	0.67	1/5859 (0.0%)
1	C	0.43	0/4682	0.66	2/6339 (0.0%)
1	D	0.42	0/4332	0.67	2/5859 (0.0%)
All	All	0.42	0/18028	0.67	7/24396 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
1	C	0	2
1	D	0	3
All	All	0	13

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	190	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	A	190	LEU	CB-CG-CD2	-6.10	100.63	111.00
1	C	513	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	513	LEU	CA-CB-CG	5.46	127.85	115.30
1	D	711	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	711	LEU	CA-CB-CG	5.36	127.62	115.30
1	D	392	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	ASP	Peptide
1	A	463	PRO	Peptide
1	A	465	GLU	Peptide
1	A	739	TRP	Peptide
1	A	89	PRO	Peptide
1	B	309	ASP	Peptide
1	B	729	ARG	Peptide
1	B	733	ARG	Peptide
1	C	739	TRP	Peptide
1	C	89	PRO	Peptide
1	D	309	ASP	Peptide
1	D	729	ARG	Peptide
1	D	733	ARG	Peptide

## 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	4581	0	4575	86	0
1	B	4239	0	4261	84	0
1	C	4581	0	4575	91	0
1	D	4239	0	4261	84	0
All	All	17640	0	17672	337	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 10.

All (337) 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:A:368:LYS:HA	1:A:371:ARG:HE	1.57	0.70
1:B:722:LYS:HD2	1:B:727:ASP:HB3	1.74	0.69
1:D:722:LYS:HD2	1:D:727:ASP:HB3	1.74	0.68
1:C:368:LYS:HA	1:C:371:ARG:HE	1.57	0.68
1:A:293:ASP:H	1:A:297:ASN:H	1.42	0.67
1:A:433:TRP:HA	1:A:437:ALA:HB3	1.77	0.67
1:C:433:TRP:HA	1:C:437:ALA:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ILE:O	1:B:416:ARG:NH2	2.28	0.66
1:B:315:ASP:O	1:B:319:ARG:NH2	2.27	0.66
1:C:395:VAL:HA	1:C:403:VAL:HG22	1.78	0.66
1:D:407:ILE:O	1:D:416:ARG:NH2	2.28	0.65
1:A:395:VAL:HA	1:A:403:VAL:HG22	1.77	0.65
1:C:293:ASP:H	1:C:297:ASN:H	1.42	0.65
1:B:260:TYR:OH	1:B:297:ASN:ND2	2.29	0.65
1:B:179:ILE:HD11	1:C:746:VAL:HG22	1.79	0.64
1:D:452:ASN:ND2	1:D:562:MET:SD	2.71	0.64
1:B:452:ASN:ND2	1:B:562:MET:SD	2.71	0.64
1:D:315:ASP:O	1:D:319:ARG:NH2	2.27	0.63
1:A:746:VAL:HG22	1:D:179:ILE:HD11	1.79	0.63
1:C:410:ASN:O	1:C:416:ARG:NH2	2.31	0.63
1:A:260:TYR:OH	1:A:297:ASN:ND2	2.32	0.63
1:C:334:GLU:OE2	1:C:363:ARG:NH2	2.32	0.63
1:A:410:ASN:O	1:A:416:ARG:NH2	2.31	0.62
1:D:260:TYR:OH	1:D:297:ASN:ND2	2.29	0.62
1:C:260:TYR:OH	1:C:297:ASN:ND2	2.33	0.62
1:C:456:THR:HG1	1:C:559:TRP:HE1	1.49	0.60
1:B:566:THR:HB	1:B:572:MET:HB3	1.83	0.60
1:B:313:GLN:HG2	1:B:315:ASP:H	1.67	0.60
1:D:716:ARG:HE	1:D:730:LEU:HD13	1.66	0.60
1:A:456:THR:HG1	1:A:559:TRP:HE1	1.48	0.59
1:D:313:GLN:HG2	1:D:315:ASP:H	1.67	0.59
1:A:337:ARG:NH1	1:A:341:GLY:O	2.35	0.59
1:A:481:TRP:HD1	1:A:484:LEU:HD12	1.68	0.59
1:B:129:GLU:O	1:B:180:ASN:ND2	2.36	0.59
1:D:566:THR:HB	1:D:572:MET:HB3	1.83	0.59
1:B:381:ALA:HA	1:B:386:SER:HA	1.85	0.58
1:D:129:GLU:O	1:D:180:ASN:ND2	2.36	0.58
1:B:564:ALA:O	1:B:567:ARG:NE	2.35	0.58
1:D:381:ALA:HA	1:D:386:SER:HA	1.86	0.58
1:C:338:ASN:OD1	1:C:342:LEU:N	2.37	0.58
1:B:716:ARG:HE	1:B:730:LEU:HD13	1.68	0.58
1:A:322:ASP:OD1	1:A:322:ASP:N	2.36	0.58
1:C:481:TRP:HD1	1:C:484:LEU:HD12	1.68	0.58
1:C:337:ARG:NH1	1:C:341:GLY:O	2.35	0.57
1:B:211:GLU:HA	1:B:214:GLU:HB3	1.85	0.57
1:D:509:ARG:HA	1:D:516:ILE:HG12	1.87	0.57
1:A:751:GLU:OE1	1:D:169:LYS:NZ	2.37	0.56
1:B:167:THR:HA	1:B:210:GLU:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:THR:HA	1:D:210:GLU:HG3	1.86	0.56
1:B:693:ARG:O	1:B:696:ARG:NH1	2.39	0.56
1:C:464:ARG:NH1	1:C:467:GLU:O	2.39	0.56
1:D:233:VAL:O	1:D:237:ALA:N	2.38	0.56
1:D:307:ALA:H	1:D:353:LYS:HZ2	1.53	0.56
1:B:509:ARG:HA	1:B:516:ILE:HG12	1.86	0.56
1:C:322:ASP:N	1:C:322:ASP:OD1	2.36	0.56
1:D:211:GLU:HA	1:D:214:GLU:HB3	1.86	0.56
1:D:364:GLU:HB3	1:D:376:LYS:HB3	1.87	0.56
1:B:364:GLU:HB3	1:B:376:LYS:HB3	1.87	0.56
1:B:267:ALA:O	1:B:271:CYS:N	2.38	0.56
1:B:346:GLN:NE2	1:B:401:ASN:O	2.39	0.56
1:D:480:SER:HB2	1:D:483:GLN:HB2	1.88	0.56
1:A:420:LEU:HD23	1:A:425:LEU:HD13	1.89	0.55
1:C:128:SER:HA	1:C:178:ASN:HD21	1.71	0.55
1:A:516:ILE:HA	1:A:520:ALA:HB3	1.88	0.55
1:D:693:ARG:O	1:D:696:ARG:NH1	2.39	0.55
1:B:480:SER:HB2	1:B:483:GLN:HB2	1.88	0.55
1:C:532:LEU:HD12	1:C:554:ALA:HB2	1.89	0.55
1:D:267:ALA:O	1:D:271:CYS:N	2.38	0.55
1:D:346:GLN:NE2	1:D:401:ASN:O	2.39	0.55
1:C:205:ASN:HD21	1:C:240:ASP:H	1.55	0.55
1:B:233:VAL:O	1:B:237:ALA:N	2.38	0.54
1:A:273:ASN:HA	1:A:320:MET:HE3	1.89	0.54
1:A:532:LEU:HD12	1:A:554:ALA:HB2	1.88	0.54
1:B:454:THR:HG21	1:B:489:PHE:HB3	1.89	0.54
1:C:420:LEU:HD23	1:C:425:LEU:HD13	1.89	0.54
1:C:516:ILE:HA	1:C:520:ALA:HB3	1.88	0.54
1:A:128:SER:HA	1:A:178:ASN:HD21	1.72	0.54
1:A:338:ASN:OD1	1:A:342:LEU:N	2.37	0.54
1:C:273:ASN:HA	1:C:320:MET:HE3	1.89	0.54
1:C:164:ALA:H	1:C:168:GLY:HA2	1.73	0.54
1:A:693:ARG:O	1:A:696:ARG:NH1	2.41	0.54
1:C:717:MET:O	1:C:732:LEU:N	2.36	0.53
1:A:205:ASN:HD21	1:A:240:ASP:H	1.55	0.53
1:D:208:TYR:HD2	1:D:214:GLU:HA	1.73	0.53
1:A:156:ASP:N	1:A:156:ASP:OD1	2.40	0.53
1:C:721:CYS:HA	1:C:728:PHE:HA	1.91	0.53
1:C:156:ASP:N	1:C:156:ASP:OD1	2.41	0.53
1:A:717:MET:O	1:A:732:LEU:N	2.35	0.53
1:A:164:ALA:H	1:A:168:GLY:HA2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:693:ARG:O	1:C:696:ARG:NH1	2.41	0.53
1:D:454:THR:HG21	1:D:489:PHE:HB3	1.90	0.53
1:D:707:LEU:HD23	1:D:711:LEU:HD13	1.90	0.53
1:D:379:ASP:N	1:D:379:ASP:OD1	2.41	0.52
1:D:361:LEU:HD13	1:D:424:PRO:HD2	1.92	0.52
1:C:226:ARG:NH1	1:D:744:THR:OG1	2.41	0.52
1:A:157:PHE:O	1:A:161:LYS:N	2.40	0.52
1:A:388:SER:HB2	1:A:735:ASN:HB2	1.91	0.52
1:C:388:SER:HB2	1:C:735:ASN:HB2	1.91	0.52
1:B:169:LYS:NZ	1:C:751:GLU:OE1	2.37	0.52
1:D:420:LEU:HA	1:D:425:LEU:HD12	1.91	0.52
1:B:253:LYS:HB2	1:B:256:HIS:HD2	1.74	0.52
1:A:721:CYS:HA	1:A:728:PHE:HA	1.91	0.52
1:B:361:LEU:HD13	1:B:424:PRO:HD2	1.92	0.52
1:C:233:VAL:O	1:C:237:ALA:N	2.36	0.52
1:C:309:ASP:OD1	1:C:415:ASN:ND2	2.43	0.52
1:D:253:LYS:HB2	1:D:256:HIS:HD2	1.74	0.52
1:B:208:TYR:HD2	1:B:214:GLU:HA	1.73	0.52
1:A:226:ARG:NH1	1:B:744:THR:OG1	2.41	0.52
1:A:208:TYR:HD2	1:A:216:GLN:HB3	1.74	0.52
1:B:707:LEU:HD23	1:B:711:LEU:HD13	1.91	0.52
1:D:176:LEU:HD12	1:D:218:ALA:HB1	1.92	0.52
1:A:309:ASP:OD1	1:A:415:ASN:ND2	2.43	0.51
1:C:208:TYR:HD2	1:C:216:GLN:HB3	1.74	0.51
1:B:268:LEU:HA	1:B:271:CYS:HB3	1.92	0.51
1:A:233:VAL:O	1:A:237:ALA:N	2.36	0.51
1:B:379:ASP:OD1	1:B:379:ASP:N	2.40	0.51
1:B:420:LEU:HA	1:B:425:LEU:HD12	1.91	0.51
1:D:448:TYR:OH	1:D:558:GLY:O	2.24	0.51
1:D:282:MET:HG3	1:D:327:ARG:HG2	1.93	0.50
1:B:212:ALA:O	1:B:248:VAL:N	2.33	0.50
1:D:268:LEU:HA	1:D:271:CYS:HB3	1.92	0.50
1:D:303:LEU:HD22	1:D:321:TYR:HD1	1.77	0.50
1:D:564:ALA:O	1:D:567:ARG:NE	2.35	0.50
1:B:176:LEU:HD12	1:B:218:ALA:HB1	1.92	0.50
1:B:282:MET:HG3	1:B:327:ARG:HG2	1.93	0.50
1:B:525:VAL:HA	1:B:528:VAL:HG22	1.94	0.50
1:C:157:PHE:O	1:C:161:LYS:N	2.39	0.50
1:C:184:LYS:HG2	1:C:230:ILE:HD11	1.94	0.50
1:A:184:LYS:HG2	1:A:230:ILE:HD11	1.94	0.49
1:A:389:LEU:HD11	1:A:732:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ALA:HB3	1:C:200:LEU:HD13	1.95	0.49
1:C:330:ASN:ND2	1:C:332:GLU:OE2	2.45	0.49
1:A:431:THR:OG1	1:A:733:ARG:NH2	2.36	0.49
1:C:389:LEU:HD11	1:C:732:LEU:HD13	1.94	0.49
1:C:431:THR:OG1	1:C:733:ARG:NH2	2.36	0.49
1:A:330:ASN:ND2	1:A:332:GLU:OE2	2.45	0.49
1:B:213:TYR:HA	1:B:247:GLY:HA3	1.94	0.49
1:D:213:TYR:HA	1:D:247:GLY:HA3	1.95	0.49
1:B:303:LEU:HD22	1:B:321:TYR:HD1	1.77	0.49
1:A:194:ALA:HB3	1:A:200:LEU:HD13	1.95	0.49
1:A:129:GLU:O	1:A:180:ASN:ND2	2.46	0.48
1:C:445:PHE:HD1	1:C:565:TYR:HB3	1.78	0.48
1:A:508:LEU:HD12	1:A:510:PRO:HD3	1.95	0.48
1:C:129:GLU:O	1:C:180:ASN:ND2	2.46	0.48
1:C:508:LEU:HD12	1:C:510:PRO:HD3	1.94	0.48
1:C:167:THR:HB	1:C:210:GLU:HB2	1.95	0.48
1:D:525:VAL:HA	1:D:528:VAL:HG22	1.94	0.48
1:C:456:THR:OG1	1:C:559:TRP:NE1	2.39	0.48
1:D:567:ARG:O	1:D:692:TRP:NE1	2.44	0.48
1:A:445:PHE:HD1	1:A:565:TYR:HB3	1.78	0.48
1:A:167:THR:HB	1:A:210:GLU:HB2	1.96	0.48
1:A:377:PHE:HB2	1:A:389:LEU:HD22	1.96	0.48
1:D:377:PHE:HB2	1:D:389:LEU:HB2	1.96	0.48
1:A:231:THR:HA	1:A:234:LEU:HD12	1.96	0.47
1:B:448:TYR:OH	1:B:558:GLY:O	2.24	0.47
1:D:212:ALA:O	1:D:248:VAL:N	2.33	0.47
1:D:298:ASN:H	1:D:301:HIS:HD2	1.62	0.47
1:A:448:TYR:OH	1:A:561:ASN:OD1	2.31	0.47
1:B:298:ASN:H	1:B:301:HIS:HD2	1.62	0.47
1:B:338:ASN:OD1	1:B:342:LEU:N	2.47	0.47
1:A:379:ASP:HB3	1:A:387:SER:HB3	1.96	0.47
1:B:231:THR:HG21	1:B:277:ILE:HD11	1.96	0.47
1:B:433:TRP:HA	1:B:437:ALA:HB3	1.96	0.47
1:D:415:ASN:HD22	1:D:418:GLU:HB3	1.80	0.47
1:D:433:TRP:HA	1:D:437:ALA:HB3	1.96	0.47
1:A:720:LEU:HB2	1:A:732:LEU:HD12	1.97	0.47
1:C:231:THR:HA	1:C:234:LEU:HD12	1.96	0.47
1:D:261:PHE:HD2	1:D:267:ALA:HB3	1.80	0.47
1:B:696:ARG:O	1:B:699:THR:OG1	2.31	0.47
1:D:387:SER:HA	1:D:734:ILE:HB	1.96	0.47
1:B:251:ASN:H	1:B:258:GLY:HA2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:GLN:HE21	1:B:316:PHE:H	1.63	0.47
1:D:497:ILE:HB	1:D:530:ALA:HB2	1.96	0.47
1:B:497:ILE:HB	1:B:530:ALA:HB2	1.96	0.47
1:B:522:PHE:O	1:B:526:PHE:N	2.46	0.47
1:B:567:ARG:O	1:B:692:TRP:NE1	2.44	0.47
1:A:696:ARG:O	1:A:699:THR:OG1	2.27	0.47
1:C:293:ASP:H	1:C:297:ASN:N	2.12	0.47
1:D:231:THR:HG21	1:D:277:ILE:HD11	1.96	0.47
1:A:456:THR:OG1	1:A:559:TRP:NE1	2.39	0.47
1:C:450:PHE:HA	1:C:453:ILE:HD12	1.97	0.47
1:D:313:GLN:HE21	1:D:316:PHE:H	1.63	0.47
1:C:377:PHE:HB2	1:C:389:LEU:HD22	1.97	0.47
1:D:340:ASP:N	1:D:340:ASP:OD1	2.38	0.47
1:A:116:LYS:O	1:A:120:LYS:N	2.46	0.46
1:B:436:PHE:HA	1:B:714:ARG:HH11	1.81	0.46
1:A:459:SER:HA	1:A:463:PRO:HG3	1.98	0.46
1:B:307:ALA:H	1:B:353:LYS:HZ2	1.63	0.46
1:D:251:ASN:H	1:D:258:GLY:HA2	1.79	0.46
1:B:415:ASN:HD22	1:B:418:GLU:HB3	1.80	0.46
1:C:448:TYR:OH	1:C:561:ASN:OD1	2.31	0.46
1:C:720:LEU:HB2	1:C:732:LEU:HD12	1.98	0.46
1:D:338:ASN:OD1	1:D:342:LEU:N	2.47	0.46
1:C:124:PHE:O	1:C:128:SER:N	2.47	0.46
1:D:195:GLU:HA	1:D:200:LEU:HD23	1.97	0.46
1:D:208:TYR:HB3	1:D:216:GLN:H	1.81	0.46
1:D:302:ALA:O	1:D:305:THR:OG1	2.31	0.46
1:D:343:THR:O	1:D:347:LEU:N	2.49	0.46
1:A:473:LEU:HG	1:A:491:LEU:HD11	1.96	0.46
1:B:208:TYR:HB3	1:B:216:GLN:H	1.81	0.46
1:D:436:PHE:HA	1:D:714:ARG:HH11	1.81	0.46
1:B:261:PHE:HD2	1:B:267:ALA:HB3	1.80	0.46
1:B:387:SER:HA	1:B:734:ILE:HB	1.97	0.46
1:C:143:GLN:O	1:C:147:ARG:N	2.48	0.46
1:A:143:GLN:O	1:A:147:ARG:N	2.48	0.46
1:B:377:PHE:HB2	1:B:389:LEU:HB2	1.97	0.46
1:C:379:ASP:HB3	1:C:387:SER:HB3	1.96	0.46
1:B:195:GLU:HA	1:B:200:LEU:HD23	1.97	0.45
1:B:379:ASP:OD1	1:B:387:SER:OG	2.26	0.45
1:C:360:ILE:HG23	1:C:363:ARG:HH21	1.80	0.45
1:C:536:SER:HA	1:C:539:LEU:HD12	1.98	0.45
1:A:450:PHE:HA	1:A:453:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PHE:O	1:A:128:SER:N	2.47	0.45
1:D:250:PHE:HB2	1:D:260:TYR:HD1	1.82	0.45
1:D:688:SER:HA	1:D:691:ILE:HD12	1.99	0.45
1:C:200:LEU:HA	1:C:203:PHE:HB3	1.98	0.45
1:C:473:LEU:HG	1:C:491:LEU:HD11	1.98	0.45
1:B:688:SER:HA	1:B:691:ILE:HD12	1.99	0.45
1:C:321:TYR:HE2	1:C:363:ARG:HH22	1.62	0.45
1:D:298:ASN:OD1	1:D:301:HIS:N	2.38	0.45
1:A:159:MET:O	1:A:163:THR:OG1	2.28	0.45
1:A:739:TRP:HD1	1:A:742:TRP:HZ2	1.65	0.45
1:C:739:TRP:HD1	1:C:742:TRP:HZ2	1.65	0.45
1:B:250:PHE:HB2	1:B:260:TYR:HD1	1.81	0.45
1:A:200:LEU:HA	1:A:203:PHE:HB3	1.98	0.45
1:A:514:GLN:O	1:A:518:SER:OG	2.35	0.45
1:C:337:ARG:HB3	1:C:341:GLY:HA2	1.99	0.45
1:D:696:ARG:O	1:D:699:THR:OG1	2.31	0.45
1:A:338:ASN:OD1	1:A:341:GLY:N	2.50	0.44
1:B:343:THR:O	1:B:347:LEU:N	2.49	0.44
1:B:318:LYS:HE3	1:B:359:TYR:HB2	2.00	0.44
1:A:293:ASP:H	1:A:297:ASN:N	2.12	0.44
1:C:338:ASN:OD1	1:C:341:GLY:N	2.50	0.44
1:A:135:LEU:HA	1:A:138:LEU:HB2	2.00	0.44
1:D:357:LEU:HA	1:D:360:ILE:HG22	2.00	0.44
1:B:391:ASP:OD2	1:B:393:THR:OG1	2.25	0.44
1:C:719:GLU:H	1:C:731:CYS:HA	1.83	0.44
1:A:536:SER:HA	1:A:539:LEU:HD12	1.99	0.43
1:A:719:GLU:H	1:A:731:CYS:HA	1.83	0.43
1:B:410:ASN:OD1	1:B:411:THR:N	2.50	0.43
1:A:337:ARG:HB3	1:A:341:GLY:HA2	1.98	0.43
1:B:448:TYR:HE2	1:B:562:MET:HA	1.83	0.43
1:A:226:ARG:HH22	1:B:744:THR:HG21	1.83	0.43
1:C:116:LYS:O	1:C:120:LYS:N	2.46	0.43
1:C:501:GLU:HA	1:C:504:ALA:HB3	2.00	0.43
1:D:318:LYS:HE3	1:D:359:TYR:HB2	2.00	0.43
1:A:274:GLN:HB3	1:A:277:ILE:HD12	2.00	0.43
1:A:732:LEU:HB3	1:A:733:ARG:H	1.61	0.43
1:B:298:ASN:OD1	1:B:301:HIS:N	2.37	0.43
1:D:313:GLN:NE2	1:D:317:VAL:H	2.16	0.43
1:D:733:ARG:HB3	1:D:734:ILE:H	1.71	0.43
1:B:313:GLN:NE2	1:B:317:VAL:H	2.16	0.43
1:C:123:ILE:O	1:C:127:VAL:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:THR:HB	1:C:730:LEU:HD23	2.01	0.43
1:D:379:ASP:OD1	1:D:387:SER:OG	2.26	0.43
1:A:272:THR:O	1:A:274:GLN:NE2	2.51	0.43
1:C:135:LEU:HA	1:C:138:LEU:HB2	2.00	0.43
1:B:392:LEU:HD12	1:B:395:VAL:HB	2.00	0.43
1:C:707:LEU:HD23	1:C:711:LEU:HG	2.00	0.43
1:D:448:TYR:HE2	1:D:562:MET:HA	1.83	0.43
1:A:365:ILE:HB	1:A:374:SER:HB2	2.00	0.43
1:A:707:LEU:HD23	1:A:711:LEU:HG	1.99	0.43
1:C:362:SER:OG	1:C:363:ARG:N	2.51	0.43
1:A:198:ASP:N	1:A:198:ASP:OD1	2.52	0.43
1:A:393:THR:HB	1:A:730:LEU:HD23	2.01	0.43
1:B:361:LEU:HD23	1:B:361:LEU:HA	1.81	0.43
1:C:470:PRO:HB2	1:C:472:PRO:HD3	2.00	0.43
1:A:707:LEU:HA	1:A:707:LEU:HD12	1.84	0.43
1:B:380:TRP:HB3	1:B:387:SER:HB3	2.01	0.43
1:C:732:LEU:HB3	1:C:733:ARG:H	1.61	0.43
1:B:307:ALA:H	1:B:353:LYS:NZ	2.17	0.43
1:B:357:LEU:HA	1:B:360:ILE:HG22	2.00	0.43
1:C:274:GLN:HB3	1:C:277:ILE:HD12	2.00	0.43
1:C:226:ARG:HH22	1:D:744:THR:HG21	1.83	0.42
1:C:514:GLN:O	1:C:518:SER:OG	2.35	0.42
1:D:380:TRP:N	1:D:387:SER:OG	2.48	0.42
1:A:162:LEU:HD11	1:A:171:CYS:H	1.84	0.42
1:C:205:ASN:ND2	1:C:240:ASP:H	2.17	0.42
1:D:522:PHE:O	1:D:526:PHE:N	2.46	0.42
1:A:546:GLU:HG2	1:A:550:CYS:HB2	2.01	0.42
1:D:410:ASN:OD1	1:D:411:THR:N	2.50	0.42
1:A:220:ASN:HA	1:A:223:ILE:HD12	2.02	0.42
1:A:486:GLY:O	1:A:490:VAL:N	2.46	0.42
1:C:162:LEU:HD11	1:C:171:CYS:H	1.85	0.42
1:C:546:GLU:HG2	1:C:550:CYS:HB2	2.02	0.42
1:D:422:LEU:HD13	1:D:422:LEU:HA	1.88	0.42
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.88	0.42
1:A:501:GLU:HA	1:A:504:ALA:HB3	2.00	0.42
1:B:224:GLU:OE1	1:B:225:ARG:NH2	2.53	0.42
1:C:180:ASN:O	1:C:183:THR:OG1	2.38	0.42
1:A:205:ASN:ND2	1:A:240:ASP:H	2.17	0.42
1:B:302:ALA:O	1:B:305:THR:OG1	2.31	0.42
1:C:177:LEU:HD23	1:C:177:LEU:HA	1.88	0.42
1:C:272:THR:O	1:C:274:GLN:NE2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:ARG:HD2	1:B:696:ARG:NH2	2.35	0.41
1:C:116:LYS:HB2	1:C:161:LYS:HE3	2.02	0.41
1:C:696:ARG:O	1:C:699:THR:OG1	2.27	0.41
1:C:135:LEU:HA	1:C:138:LEU:HD12	2.02	0.41
1:C:325:LEU:HA	1:C:325:LEU:HD13	1.90	0.41
1:D:410:ASN:ND2	1:D:413:ILE:HD13	2.35	0.41
1:A:448:TYR:OH	1:A:558:GLY:O	2.37	0.41
1:B:241:VAL:HG21	1:B:287:THR:HA	2.01	0.41
1:C:448:TYR:OH	1:C:558:GLY:O	2.37	0.41
1:D:241:VAL:HG21	1:D:287:THR:HA	2.01	0.41
1:A:360:ILE:HG23	1:A:363:ARG:NH2	2.35	0.41
1:A:688:SER:HA	1:A:691:ILE:HD12	2.03	0.41
1:C:123:ILE:HG13	1:C:138:LEU:HD22	2.02	0.41
1:D:224:GLU:OE1	1:D:225:ARG:NH2	2.53	0.41
1:D:693:ARG:HD2	1:D:696:ARG:NH2	2.35	0.41
1:A:180:ASN:O	1:A:183:THR:OG1	2.38	0.41
1:B:400:ASP:N	1:B:400:ASP:OD1	2.53	0.41
1:B:693:ARG:HD2	1:B:696:ARG:HH21	1.86	0.41
1:C:220:ASN:HA	1:C:223:ILE:HD12	2.02	0.41
1:A:362:SER:OG	1:A:363:ARG:N	2.54	0.41
1:B:176:LEU:HA	1:B:176:LEU:HD23	1.83	0.41
1:D:176:LEU:HA	1:D:176:LEU:HD23	1.83	0.41
1:C:332:GLU:O	1:C:335:THR:OG1	2.32	0.41
1:D:307:ALA:H	1:D:353:LYS:NZ	2.17	0.41
1:A:135:LEU:HA	1:A:138:LEU:HD12	2.02	0.41
1:B:733:ARG:HB3	1:B:734:ILE:H	1.77	0.41
1:C:563:LEU:HA	1:C:566:THR:HG22	2.03	0.41
1:A:563:LEU:HA	1:A:566:THR:HG22	2.03	0.41
1:B:380:TRP:N	1:B:387:SER:OG	2.47	0.41
1:D:292:GLN:HB3	1:D:296:GLY:HA2	2.03	0.41
1:B:410:ASN:ND2	1:B:413:ILE:HD13	2.35	0.40
1:C:365:ILE:HB	1:C:374:SER:HB2	2.02	0.40
1:D:380:TRP:HB3	1:D:387:SER:HB3	2.03	0.40
1:D:390:TYR:CG	1:D:424:PRO:HG3	2.56	0.40
1:A:295:ARG:HB3	1:A:297:ASN:ND2	2.37	0.40
1:D:400:ASP:OD1	1:D:400:ASP:N	2.53	0.40
1:B:390:TYR:CG	1:B:424:PRO:HG3	2.57	0.40
1:C:361:LEU:HD21	1:C:424:PRO:HG2	2.04	0.40
1:D:264:THR:HA	1:D:265:PRO:HD3	1.95	0.40
1:B:698:ARG:HD2	1:B:698:ARG:HA	1.94	0.40
1:C:172:LEU:HA	1:C:172:LEU:HD13	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ASN:HA	1:C:301:HIS:HD1	1.87	0.40
1:D:437:ALA:HB2	1:D:700:ILE:HD13	2.04	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	558/808 (69%)	475 (85%)	82 (15%)	1 (0%)	49	84
1	B	514/808 (64%)	438 (85%)	73 (14%)	3 (1%)	27	68
1	C	558/808 (69%)	476 (85%)	81 (14%)	1 (0%)	49	84
1	D	514/808 (64%)	438 (85%)	73 (14%)	3 (1%)	27	68
All	All	2144/3232 (66%)	1827 (85%)	309 (14%)	8 (0%)	40	76

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	412	ASN
1	D	412	ASN
1	A	113	ARG
1	C	113	ARG
1	B	411	THR
1	D	411	THR
1	D	413	ILE
1	B	413	ILE

### 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	499/720 (69%)	491 (98%)	8 (2%)	65	83
1	B	458/720 (64%)	443 (97%)	15 (3%)	41	68
1	C	499/720 (69%)	491 (98%)	8 (2%)	65	83
1	D	458/720 (64%)	443 (97%)	15 (3%)	41	68
All	All	1914/2880 (66%)	1868 (98%)	46 (2%)	55	75

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ARG
1	A	149	ARG
1	A	202	ARG
1	A	246	LYS
1	A	401	ASN
1	A	545	LYS
1	A	696	ARG
1	A	716	ARG
1	B	118	ARG
1	B	178	ASN
1	B	197	ASN
1	B	220	ASN
1	B	272	THR
1	B	306	VAL
1	B	314	ASN
1	B	342	LEU
1	B	366	LYS
1	B	401	ASN
1	B	462	ARG
1	B	479	MET
1	B	483	GLN
1	B	696	ARG
1	B	716	ARG
1	C	113	ARG
1	C	149	ARG
1	C	202	ARG
1	C	246	LYS
1	C	401	ASN

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Mol	Chain	Res	Type
1	C	545	LYS
1	C	696	ARG
1	C	716	ARG
1	D	118	ARG
1	D	178	ASN
1	D	197	ASN
1	D	220	ASN
1	D	272	THR
1	D	306	VAL
1	D	314	ASN
1	D	342	LEU
1	D	366	LYS
1	D	401	ASN
1	D	462	ARG
1	D	479	MET
1	D	483	GLN
1	D	696	ARG
1	D	716	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	255	GLN
1	A	297	ASN
1	A	401	ASN
1	B	178	ASN
1	B	220	ASN
1	B	256	HIS
1	B	297	ASN
1	B	301	HIS
1	B	313	GLN
1	B	314	ASN
1	B	401	ASN
1	B	452	ASN
1	B	735	ASN
1	C	205	ASN
1	C	255	GLN
1	C	297	ASN
1	C	401	ASN
1	D	178	ASN
1	D	220	ASN

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Mol	Chain	Res	Type
1	D	256	HIS
1	D	297	ASN
1	D	301	HIS
1	D	313	GLN
1	D	314	ASN
1	D	401	ASN
1	D	452	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 ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.