



# Full wwPDB EM Validation Report (i)

Oct 22, 2024 – 12:25 AM JST

PDB ID : 8K1D  
EMDB ID : EMD-36792  
Title : SID1 transmembrane family member 1  
Authors : Guo, H.; Qi, C.; Lu, Y.; Yang, H.; Zhu, Y.; Sun, F.; Ji, X.  
Deposited on : 2023-07-10  
Resolution : 3.53 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 (i) symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references \(i\)](#)) were used in the production of this report:

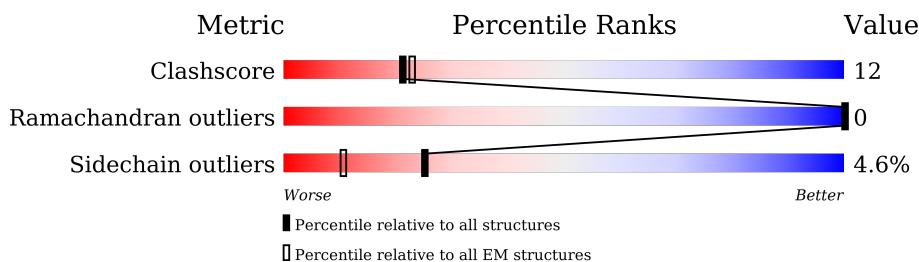
EMDB validation analysis : **FAILED**  
MolProbitY : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
**ELECTRON MICROSCOPY**

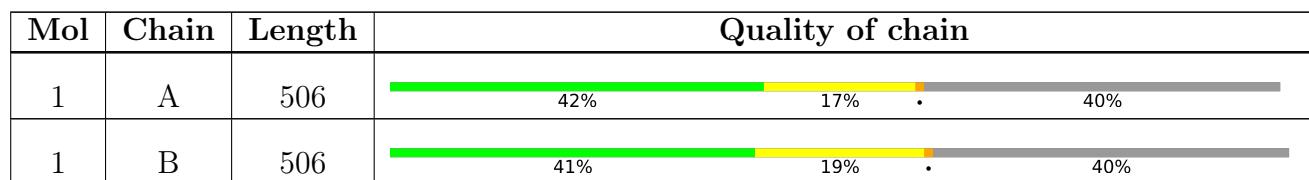
The reported resolution of this entry is 3.53 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%



## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4902 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 SID1 transmembrane family member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	305	2451	1655	379	398	19	0	0
1	B	305	2451	1655	379	398	19	0	0

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP Q9NXL6
A	?	-	SER	deletion	UNP Q9NXL6
A	?	-	ASN	deletion	UNP Q9NXL6
A	?	-	TYR	deletion	UNP Q9NXL6
A	?	-	GLY	deletion	UNP Q9NXL6
A	?	-	THR	deletion	UNP Q9NXL6
A	?	-	ILE	deletion	UNP Q9NXL6
A	?	-	ASP	deletion	UNP Q9NXL6
A	?	-	GLU	deletion	UNP Q9NXL6
A	?	-	SER	deletion	UNP Q9NXL6
A	?	-	SER	deletion	UNP Q9NXL6
A	?	-	SER	deletion	UNP Q9NXL6
A	?	-	PRO	deletion	UNP Q9NXL6
A	?	-	GLY	deletion	UNP Q9NXL6
A	?	-	ARG	deletion	UNP Q9NXL6
A	?	-	GLN	deletion	UNP Q9NXL6
A	?	-	MET	deletion	UNP Q9NXL6
A	?	-	SER	deletion	UNP Q9NXL6
A	?	-	SER	deletion	UNP Q9NXL6
A	?	-	SER	deletion	UNP Q9NXL6
A	?	-	ASP	deletion	UNP Q9NXL6
A	?	-	GLY	deletion	UNP Q9NXL6
A	?	-	GLY	deletion	UNP Q9NXL6
A	?	-	PRO	deletion	UNP Q9NXL6
A	?	-	PRO	deletion	UNP Q9NXL6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP Q9NXL6
A	?	-	GLN	deletion	UNP Q9NXL6
A	?	-	SER	deletion	UNP Q9NXL6
A	?	-	ASP	deletion	UNP Q9NXL6
A	?	-	THR	deletion	UNP Q9NXL6
A	?	-	ASP	deletion	UNP Q9NXL6
A	?	-	SER	deletion	UNP Q9NXL6
A	?	-	SER	deletion	UNP Q9NXL6
A	?	-	VAL	deletion	UNP Q9NXL6
A	?	-	GLU	deletion	UNP Q9NXL6
A	?	-	GLU	deletion	UNP Q9NXL6
A	?	-	SER	deletion	UNP Q9NXL6
A	?	-	ASP	deletion	UNP Q9NXL6
A	?	-	PHE	deletion	UNP Q9NXL6
A	?	-	ASP	deletion	UNP Q9NXL6
A	?	-	THR	deletion	UNP Q9NXL6
A	?	-	MET	deletion	UNP Q9NXL6
A	828	ASP	-	expression tag	UNP Q9NXL6
A	829	TYR	-	expression tag	UNP Q9NXL6
A	830	LYS	-	expression tag	UNP Q9NXL6
A	831	ASP	-	expression tag	UNP Q9NXL6
A	832	HIS	-	expression tag	UNP Q9NXL6
A	833	ASP	-	expression tag	UNP Q9NXL6
A	834	GLY	-	expression tag	UNP Q9NXL6
A	835	ASP	-	expression tag	UNP Q9NXL6
A	836	TYR	-	expression tag	UNP Q9NXL6
A	837	LYS	-	expression tag	UNP Q9NXL6
A	838	ASP	-	expression tag	UNP Q9NXL6
A	839	HIS	-	expression tag	UNP Q9NXL6
A	840	ASP	-	expression tag	UNP Q9NXL6
A	841	ILE	-	expression tag	UNP Q9NXL6
A	842	ASP	-	expression tag	UNP Q9NXL6
A	843	TYR	-	expression tag	UNP Q9NXL6
A	844	LYS	-	expression tag	UNP Q9NXL6
A	845	ASP	-	expression tag	UNP Q9NXL6
A	846	ASP	-	expression tag	UNP Q9NXL6
A	847	ASP	-	expression tag	UNP Q9NXL6
A	848	ASP	-	expression tag	UNP Q9NXL6
A	849	LYS	-	expression tag	UNP Q9NXL6
B	?	-	GLY	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	ASN	deletion	UNP Q9NXL6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	deletion	UNP Q9NXL6
B	?	-	GLY	deletion	UNP Q9NXL6
B	?	-	THR	deletion	UNP Q9NXL6
B	?	-	ILE	deletion	UNP Q9NXL6
B	?	-	ASP	deletion	UNP Q9NXL6
B	?	-	GLU	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	PRO	deletion	UNP Q9NXL6
B	?	-	GLY	deletion	UNP Q9NXL6
B	?	-	ARG	deletion	UNP Q9NXL6
B	?	-	GLN	deletion	UNP Q9NXL6
B	?	-	MET	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	ASP	deletion	UNP Q9NXL6
B	?	-	GLY	deletion	UNP Q9NXL6
B	?	-	GLY	deletion	UNP Q9NXL6
B	?	-	PRO	deletion	UNP Q9NXL6
B	?	-	PRO	deletion	UNP Q9NXL6
B	?	-	GLY	deletion	UNP Q9NXL6
B	?	-	GLN	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	ASP	deletion	UNP Q9NXL6
B	?	-	THR	deletion	UNP Q9NXL6
B	?	-	ASP	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	VAL	deletion	UNP Q9NXL6
B	?	-	GLU	deletion	UNP Q9NXL6
B	?	-	GLU	deletion	UNP Q9NXL6
B	?	-	SER	deletion	UNP Q9NXL6
B	?	-	ASP	deletion	UNP Q9NXL6
B	?	-	PHE	deletion	UNP Q9NXL6
B	?	-	ASP	deletion	UNP Q9NXL6
B	?	-	THR	deletion	UNP Q9NXL6
B	?	-	MET	deletion	UNP Q9NXL6
B	828	ASP	-	expression tag	UNP Q9NXL6
B	829	TYR	-	expression tag	UNP Q9NXL6

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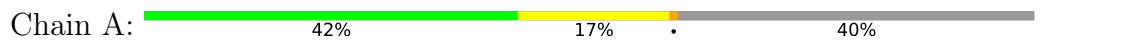
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Chain	Residue	Modelled	Actual	Comment	Reference
B	830	LYS	-	expression tag	UNP Q9NXL6
B	831	ASP	-	expression tag	UNP Q9NXL6
B	832	HIS	-	expression tag	UNP Q9NXL6
B	833	ASP	-	expression tag	UNP Q9NXL6
B	834	GLY	-	expression tag	UNP Q9NXL6
B	835	ASP	-	expression tag	UNP Q9NXL6
B	836	TYR	-	expression tag	UNP Q9NXL6
B	837	LYS	-	expression tag	UNP Q9NXL6
B	838	ASP	-	expression tag	UNP Q9NXL6
B	839	HIS	-	expression tag	UNP Q9NXL6
B	840	ASP	-	expression tag	UNP Q9NXL6
B	841	ILE	-	expression tag	UNP Q9NXL6
B	842	ASP	-	expression tag	UNP Q9NXL6
B	843	TYR	-	expression tag	UNP Q9NXL6
B	844	LYS	-	expression tag	UNP Q9NXL6
B	845	ASP	-	expression tag	UNP Q9NXL6
B	846	ASP	-	expression tag	UNP Q9NXL6
B	847	ASP	-	expression tag	UNP Q9NXL6
B	848	ASP	-	expression tag	UNP Q9NXL6
B	849	LYS	-	expression tag	UNP Q9NXL6

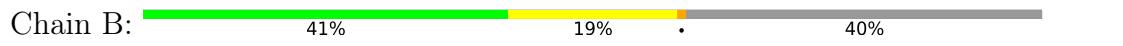
### 3 Residue-property plots

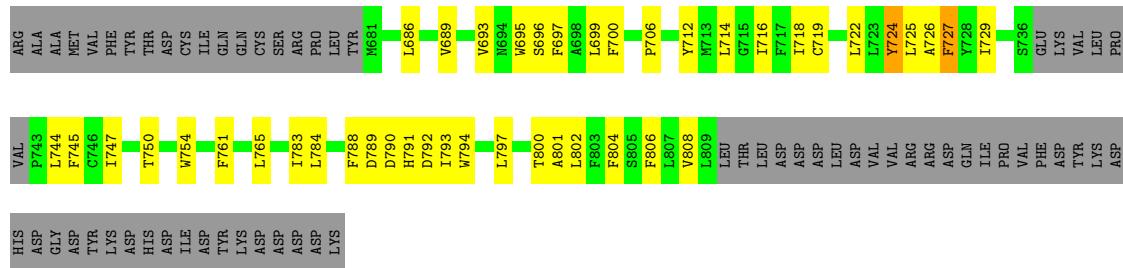
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: SID1 transmembrane family member 1



- Molecule 1: SID1 transmembrane family member 1





## 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81463	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

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	0.26	0/2521	0.49	0/3423
1	B	0.27	0/2521	0.51	0/3423
All	All	0.27	0/5042	0.50	0/6846

There are no bond length outliers.

There are no bond angle outliers.

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	2451	0	2441	53	0
1	B	2451	0	2441	60	0
All	All	4902	0	4882	113	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 12.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ( $\text{\AA}$ )	Clash overlap ( $\text{\AA}$ )
1:B:514:ILE:HG22	1:B:517:ARG:HE	1.46	0.78
1:A:448:ILE:HD12	1:A:451:ILE:HD11	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:SER:O	1:A:802:LEU:HG	1.89	0.71
1:A:790:ASP:HA	1:A:793:ILE:HD12	1.74	0.70
1:B:321:TYR:CE1	1:B:510:LEU:HB2	2.27	0.70
1:B:321:TYR:HE1	1:B:510:LEU:HB2	1.56	0.67
1:B:784:LEU:HB3	1:B:788:PHE:HB2	1.76	0.66
1:B:802:LEU:HG	1:B:806:PHE:CE2	2.31	0.66
1:A:473:THR:HG23	1:A:475:ASN:H	1.60	0.65
1:B:482:ASN:ND2	1:B:789:ASP:OD1	2.31	0.63
1:A:797:LEU:HA	1:A:800:THR:HG22	1.80	0.62
1:A:761:PHE:HB2	1:A:794:TRP:CE3	2.35	0.62
1:B:797:LEU:HA	1:B:800:THR:HG22	1.81	0.61
1:A:510:LEU:O	1:A:514:ILE:HG12	2.00	0.61
1:B:790:ASP:HA	1:B:793:ILE:HD12	1.82	0.60
1:A:784:LEU:HB3	1:A:788:PHE:HB2	1.82	0.60
1:A:310:SER:O	1:A:314:VAL:HG23	2.01	0.60
1:B:580:MET:O	1:B:584:LEU:HG	2.01	0.60
1:A:793:ILE:O	1:A:797:LEU:HD12	2.01	0.59
1:B:496:ASN:ND2	1:B:497:ASN:OD1	2.36	0.59
1:B:510:LEU:O	1:B:514:ILE:HG12	2.02	0.59
1:A:460:ILE:H	1:A:460:ILE:HD12	1.68	0.58
1:A:580:MET:O	1:A:584:LEU:HG	2.03	0.57
1:A:304:SER:O	1:A:308:LYS:HG3	2.04	0.57
1:B:744:LEU:HD12	1:B:747:ILE:HD12	1.87	0.56
1:B:712:TYR:O	1:B:716:ILE:HG23	2.06	0.56
1:A:447:ASN:O	1:A:451:ILE:HG12	2.07	0.55
1:A:508:GLY:O	1:A:512:LEU:HG	2.05	0.55
1:A:513:LEU:O	1:A:517:ARG:HG2	2.07	0.55
1:A:321:TYR:CD1	1:A:510:LEU:HD12	2.42	0.54
1:A:749:ALA:O	1:A:753:MET:HG2	2.07	0.54
1:A:519:ASP:O	1:A:523:ARG:HG3	2.08	0.53
1:A:459:VAL:O	1:A:463:VAL:HG12	2.09	0.53
1:B:456:ALA:O	1:B:460:ILE:HG12	2.07	0.53
1:B:478:ILE:O	1:B:567:ASN:ND2	2.42	0.53
1:B:519:ASP:O	1:B:523:ARG:HG3	2.09	0.52
1:B:714:LEU:O	1:B:718:ILE:HG22	2.09	0.52
1:A:311:LEU:HG	1:A:315:PHE:HD2	1.75	0.52
1:B:747:ILE:O	1:B:750:THR:OG1	2.28	0.52
1:B:459:VAL:O	1:B:463:VAL:HG12	2.09	0.52
1:A:478:ILE:O	1:A:567:ASN:ND2	2.43	0.52
1:B:469:VAL:O	1:B:473:THR:OG1	2.23	0.52
1:B:315:PHE:HA	1:B:318:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:O	1:A:326:LEU:HD22	2.11	0.51
1:A:456:ALA:O	1:A:460:ILE:HD12	2.10	0.51
1:A:498:ILE:HD11	1:A:564:VAL:HG22	1.93	0.51
1:A:754:TRP:CD1	1:A:801:ALA:HB1	2.45	0.51
1:B:310:SER:O	1:B:314:VAL:HG12	2.10	0.51
1:B:501:ASN:ND2	1:B:559:SER:OG	2.43	0.51
1:B:456:ALA:O	1:B:459:VAL:HG22	2.11	0.51
1:A:806:PHE:HD1	1:A:809:LEU:HD12	1.75	0.51
1:B:793:ILE:O	1:B:797:LEU:HD22	2.11	0.51
1:A:313:SER:O	1:A:316:ILE:HG13	2.10	0.50
1:B:311:LEU:HG	1:B:315:PHE:HD2	1.76	0.50
1:B:455:TYR:OH	1:B:573:PHE:O	2.30	0.50
1:A:644:SER:OG	1:A:724:TYR:OH	2.27	0.49
1:B:761:PHE:HB2	1:B:794:TRP:CE3	2.47	0.49
1:B:804:PHE:O	1:B:808:VAL:HG23	2.14	0.47
1:A:317:PHE:HA	1:A:320:PHE:HD2	1.80	0.47
1:B:697:PHE:HA	1:B:700:PHE:CD2	2.50	0.47
1:A:804:PHE:O	1:A:808:VAL:HG23	2.14	0.46
1:B:706:PRO:HG3	1:B:712:TYR:CD2	2.49	0.46
1:A:753:MET:SD	1:A:753:MET:N	2.87	0.46
1:B:754:TRP:CD1	1:B:801:ALA:HB1	2.50	0.46
1:A:756:ALA:HB3	1:A:797:LEU:HD22	1.98	0.46
1:A:496:ASN:ND2	1:A:497:ASN:OD1	2.48	0.46
1:B:302:LYS:HD3	1:B:302:LYS:HA	1.73	0.46
1:A:519:ASP:OD2	1:A:523:ARG:NH2	2.47	0.46
1:A:725:LEU:HD12	1:A:725:LEU:HA	1.82	0.46
1:A:746:CYS:O	1:A:750:THR:HG23	2.15	0.46
1:B:519:ASP:OD2	1:B:523:ARG:NH2	2.48	0.46
1:A:794:TRP:O	1:A:798:SER:OG	2.30	0.45
1:A:744:LEU:HD12	1:A:747:ILE:HD12	1.99	0.45
1:B:802:LEU:HG	1:B:806:PHE:HE2	1.77	0.45
1:B:554:MET:HA	1:B:557:VAL:HG12	2.00	0.44
1:B:726:ALA:HA	1:B:729:ILE:HG12	1.99	0.44
1:B:765:LEU:HD21	1:B:791:HIS:HB2	1.98	0.44
1:A:553:MET:HB3	1:A:554:MET:HE3	2.00	0.44
1:B:686:LEU:HD13	1:B:727:PHE:CZ	2.52	0.43
1:B:793:ILE:HG22	1:B:797:LEU:CD2	2.49	0.43
1:A:686:LEU:HD13	1:A:727:PHE:CZ	2.53	0.43
1:B:500:SER:HB3	1:B:788:PHE:HE2	1.83	0.43
1:B:637:VAL:HG13	1:B:695:TRP:HE1	1.83	0.43
1:A:712:TYR:O	1:A:716:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:PHE:HA	1:B:548:MET:HG3	2.00	0.43
1:B:558:LEU:HD22	1:B:574:ASP:HA	2.01	0.43
1:A:305:VAL:HA	1:A:308:LYS:HE2	2.01	0.42
1:A:554:MET:HA	1:A:557:VAL:HG12	2.00	0.42
1:B:304:SER:O	1:B:308:LYS:HG3	2.20	0.42
1:B:485:CYS:SG	1:B:789:ASP:HB3	2.59	0.42
1:B:644:SER:OG	1:B:724:TYR:OH	2.29	0.42
1:B:725:LEU:O	1:B:729:ILE:HG23	2.20	0.42
1:B:571:PHE:O	1:B:575:THR:HG22	2.20	0.41
1:B:693:VAL:O	1:B:696:SER:OG	2.35	0.41
1:A:689:VAL:O	1:A:693:VAL:HG22	2.19	0.41
1:B:507:LEU:HD23	1:B:507:LEU:HA	1.86	0.41
1:A:469:VAL:HA	1:A:472:VAL:HG22	2.02	0.41
1:A:505:VAL:HG23	1:A:553:MET:SD	2.60	0.41
1:B:461:GLN:O	1:B:464:ILE:HG22	2.20	0.41
1:A:302:LYS:HD3	1:A:302:LYS:HA	1.75	0.41
1:B:689:VAL:O	1:B:693:VAL:HG22	2.20	0.41
1:B:719:CYS:O	1:B:722:LEU:HG	2.21	0.41
1:B:783:ILE:HD12	1:B:783:ILE:HA	1.86	0.41
1:A:784:LEU:HG	1:A:785:LEU:HG	2.02	0.41
1:A:637:VAL:HG13	1:A:695:TRP:HE1	1.85	0.40
1:B:448:ILE:HA	1:B:451:ILE:HG22	2.02	0.40
1:B:455:TYR:O	1:B:458:PRO:HD2	2.21	0.40
1:A:571:PHE:O	1:A:575:THR:HG22	2.21	0.40
1:B:696:SER:HB2	1:B:700:PHE:CZ	2.56	0.40
1:A:303:GLU:HA	1:A:306:TYR:CD1	2.57	0.40
1:B:696:SER:O	1:B:699:LEU:HG	2.21	0.40
1:A:793:ILE:HG22	1:A:797:LEU:CD1	2.52	0.40
1:B:477:ASP:OD1	1:B:477:ASP:N	2.54	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	293/506 (58%)	288 (98%)	5 (2%)	0	100 100
1	B	293/506 (58%)	290 (99%)	3 (1%)	0	100 100
All	All	586/1012 (58%)	578 (99%)	8 (1%)	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	261/447 (58%)	251 (96%)	10 (4%)	28 57
1	B	261/447 (58%)	247 (95%)	14 (5%)	18 47
All	All	522/894 (58%)	498 (95%)	24 (5%)	25 52

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

Mol	Chain	Res	Type
1	A	315	PHE
1	A	455	TYR
1	A	466	TYR
1	A	485	CYS
1	A	724	TYR
1	A	727	PHE
1	A	745	PHE
1	A	762	PHE
1	A	792	ASP
1	A	794	TRP
1	B	303	GLU
1	B	315	PHE
1	B	320	PHE
1	B	445	PHE
1	B	455	TYR
1	B	466	TYR
1	B	485	CYS
1	B	509	PHE

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Mol	Chain	Res	Type
1	B	542	PHE
1	B	577	PHE
1	B	724	TYR
1	B	727	PHE
1	B	745	PHE
1	B	792	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

### 5.5 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

### 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.