



Full wwPDB EM Validation Report ⓘ

Nov 30, 2025 – 12:18 AM JST

PDB ID : 9ISG / pdb_00009isg
EMDB ID : EMD-60835
Title : Structure of rat TRPV1 in complex with PSFL426-S5
Authors : Chen, X.; Yu, Y.
Deposited on : 2024-07-17
Resolution : 3.50 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

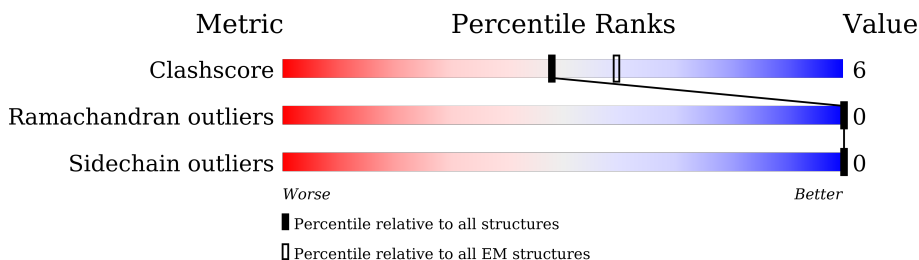
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	879	<div> <div>50%</div> <div>10%</div> <div>40%</div> </div>
1	B	879	<div> <div>52%</div> <div>9%</div> <div>40%</div> </div>
1	C	879	<div> <div>51%</div> <div>9%</div> <div>40%</div> </div>
1	D	879	<div> <div>52%</div> <div>9%</div> <div>40%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34488 atoms, of which 17268 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 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	528	Total	C	H	N	O	S	0	0
			8610	2817	4315	690	763	25		
1	B	528	Total	C	H	N	O	S	0	0
			8610	2817	4315	690	763	25		
1	C	528	Total	C	H	N	O	S	0	0
			8610	2817	4315	690	763	25		
1	D	528	Total	C	H	N	O	S	0	0
			8610	2817	4315	690	763	25		

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	initiating methionine	UNP O35433
A	-39	ASP	-	expression tag	UNP O35433
A	-38	TYR	-	expression tag	UNP O35433
A	-37	LYS	-	expression tag	UNP O35433
A	-36	ASP	-	expression tag	UNP O35433
A	-35	ASP	-	expression tag	UNP O35433
A	-34	ASP	-	expression tag	UNP O35433
A	-33	ASP	-	expression tag	UNP O35433
A	-32	LYS	-	expression tag	UNP O35433
A	-31	TRP	-	expression tag	UNP O35433
A	-30	SER	-	expression tag	UNP O35433
A	-29	HIS	-	expression tag	UNP O35433
A	-28	PRO	-	expression tag	UNP O35433
A	-27	GLN	-	expression tag	UNP O35433
A	-26	PHE	-	expression tag	UNP O35433
A	-25	GLU	-	expression tag	UNP O35433
A	-24	LYS	-	expression tag	UNP O35433
A	-23	GLY	-	expression tag	UNP O35433
A	-22	GLY	-	expression tag	UNP O35433
A	-21	GLY	-	expression tag	UNP O35433
A	-20	GLY	-	expression tag	UNP O35433

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	SER	-	expression tag	UNP O35433
A	-18	GLY	-	expression tag	UNP O35433
A	-17	GLY	-	expression tag	UNP O35433
A	-16	SER	-	expression tag	UNP O35433
A	-15	ALA	-	expression tag	UNP O35433
A	-14	TRP	-	expression tag	UNP O35433
A	-13	SER	-	expression tag	UNP O35433
A	-12	HIS	-	expression tag	UNP O35433
A	-11	PRO	-	expression tag	UNP O35433
A	-10	GLN	-	expression tag	UNP O35433
A	-9	PHE	-	expression tag	UNP O35433
A	-8	GLU	-	expression tag	UNP O35433
A	-7	LYS	-	expression tag	UNP O35433
A	-6	GLU	-	expression tag	UNP O35433
A	-5	PHE	-	expression tag	UNP O35433
A	-4	LYS	-	expression tag	UNP O35433
A	-3	GLY	-	expression tag	UNP O35433
A	-2	LEU	-	expression tag	UNP O35433
A	-1	VAL	-	expression tag	UNP O35433
A	0	ASP	-	expression tag	UNP O35433
B	-40	MET	-	initiating methionine	UNP O35433
B	-39	ASP	-	expression tag	UNP O35433
B	-38	TYR	-	expression tag	UNP O35433
B	-37	LYS	-	expression tag	UNP O35433
B	-36	ASP	-	expression tag	UNP O35433
B	-35	ASP	-	expression tag	UNP O35433
B	-34	ASP	-	expression tag	UNP O35433
B	-33	ASP	-	expression tag	UNP O35433
B	-32	LYS	-	expression tag	UNP O35433
B	-31	TRP	-	expression tag	UNP O35433
B	-30	SER	-	expression tag	UNP O35433
B	-29	HIS	-	expression tag	UNP O35433
B	-28	PRO	-	expression tag	UNP O35433
B	-27	GLN	-	expression tag	UNP O35433
B	-26	PHE	-	expression tag	UNP O35433
B	-25	GLU	-	expression tag	UNP O35433
B	-24	LYS	-	expression tag	UNP O35433
B	-23	GLY	-	expression tag	UNP O35433
B	-22	GLY	-	expression tag	UNP O35433
B	-21	GLY	-	expression tag	UNP O35433
B	-20	GLY	-	expression tag	UNP O35433
B	-19	SER	-	expression tag	UNP O35433

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP O35433
B	-17	GLY	-	expression tag	UNP O35433
B	-16	SER	-	expression tag	UNP O35433
B	-15	ALA	-	expression tag	UNP O35433
B	-14	TRP	-	expression tag	UNP O35433
B	-13	SER	-	expression tag	UNP O35433
B	-12	HIS	-	expression tag	UNP O35433
B	-11	PRO	-	expression tag	UNP O35433
B	-10	GLN	-	expression tag	UNP O35433
B	-9	PHE	-	expression tag	UNP O35433
B	-8	GLU	-	expression tag	UNP O35433
B	-7	LYS	-	expression tag	UNP O35433
B	-6	GLU	-	expression tag	UNP O35433
B	-5	PHE	-	expression tag	UNP O35433
B	-4	LYS	-	expression tag	UNP O35433
B	-3	GLY	-	expression tag	UNP O35433
B	-2	LEU	-	expression tag	UNP O35433
B	-1	VAL	-	expression tag	UNP O35433
B	0	ASP	-	expression tag	UNP O35433
C	-40	MET	-	initiating methionine	UNP O35433
C	-39	ASP	-	expression tag	UNP O35433
C	-38	TYR	-	expression tag	UNP O35433
C	-37	LYS	-	expression tag	UNP O35433
C	-36	ASP	-	expression tag	UNP O35433
C	-35	ASP	-	expression tag	UNP O35433
C	-34	ASP	-	expression tag	UNP O35433
C	-33	ASP	-	expression tag	UNP O35433
C	-32	LYS	-	expression tag	UNP O35433
C	-31	TRP	-	expression tag	UNP O35433
C	-30	SER	-	expression tag	UNP O35433
C	-29	HIS	-	expression tag	UNP O35433
C	-28	PRO	-	expression tag	UNP O35433
C	-27	GLN	-	expression tag	UNP O35433
C	-26	PHE	-	expression tag	UNP O35433
C	-25	GLU	-	expression tag	UNP O35433
C	-24	LYS	-	expression tag	UNP O35433
C	-23	GLY	-	expression tag	UNP O35433
C	-22	GLY	-	expression tag	UNP O35433
C	-21	GLY	-	expression tag	UNP O35433
C	-20	GLY	-	expression tag	UNP O35433
C	-19	SER	-	expression tag	UNP O35433
C	-18	GLY	-	expression tag	UNP O35433

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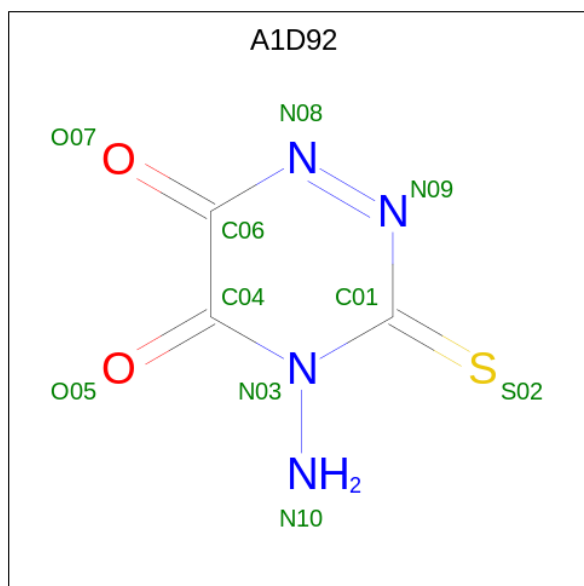
Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	GLY	-	expression tag	UNP O35433
C	-16	SER	-	expression tag	UNP O35433
C	-15	ALA	-	expression tag	UNP O35433
C	-14	TRP	-	expression tag	UNP O35433
C	-13	SER	-	expression tag	UNP O35433
C	-12	HIS	-	expression tag	UNP O35433
C	-11	PRO	-	expression tag	UNP O35433
C	-10	GLN	-	expression tag	UNP O35433
C	-9	PHE	-	expression tag	UNP O35433
C	-8	GLU	-	expression tag	UNP O35433
C	-7	LYS	-	expression tag	UNP O35433
C	-6	GLU	-	expression tag	UNP O35433
C	-5	PHE	-	expression tag	UNP O35433
C	-4	LYS	-	expression tag	UNP O35433
C	-3	GLY	-	expression tag	UNP O35433
C	-2	LEU	-	expression tag	UNP O35433
C	-1	VAL	-	expression tag	UNP O35433
C	0	ASP	-	expression tag	UNP O35433
D	-40	MET	-	initiating methionine	UNP O35433
D	-39	ASP	-	expression tag	UNP O35433
D	-38	TYR	-	expression tag	UNP O35433
D	-37	LYS	-	expression tag	UNP O35433
D	-36	ASP	-	expression tag	UNP O35433
D	-35	ASP	-	expression tag	UNP O35433
D	-34	ASP	-	expression tag	UNP O35433
D	-33	ASP	-	expression tag	UNP O35433
D	-32	LYS	-	expression tag	UNP O35433
D	-31	TRP	-	expression tag	UNP O35433
D	-30	SER	-	expression tag	UNP O35433
D	-29	HIS	-	expression tag	UNP O35433
D	-28	PRO	-	expression tag	UNP O35433
D	-27	GLN	-	expression tag	UNP O35433
D	-26	PHE	-	expression tag	UNP O35433
D	-25	GLU	-	expression tag	UNP O35433
D	-24	LYS	-	expression tag	UNP O35433
D	-23	GLY	-	expression tag	UNP O35433
D	-22	GLY	-	expression tag	UNP O35433
D	-21	GLY	-	expression tag	UNP O35433
D	-20	GLY	-	expression tag	UNP O35433
D	-19	SER	-	expression tag	UNP O35433
D	-18	GLY	-	expression tag	UNP O35433
D	-17	GLY	-	expression tag	UNP O35433

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP O35433
D	-15	ALA	-	expression tag	UNP O35433
D	-14	TRP	-	expression tag	UNP O35433
D	-13	SER	-	expression tag	UNP O35433
D	-12	HIS	-	expression tag	UNP O35433
D	-11	PRO	-	expression tag	UNP O35433
D	-10	GLN	-	expression tag	UNP O35433
D	-9	PHE	-	expression tag	UNP O35433
D	-8	GLU	-	expression tag	UNP O35433
D	-7	LYS	-	expression tag	UNP O35433
D	-6	GLU	-	expression tag	UNP O35433
D	-5	PHE	-	expression tag	UNP O35433
D	-4	LYS	-	expression tag	UNP O35433
D	-3	GLY	-	expression tag	UNP O35433
D	-2	LEU	-	expression tag	UNP O35433
D	-1	VAL	-	expression tag	UNP O35433
D	0	ASP	-	expression tag	UNP O35433

- Molecule 2 is 4-azanyl-3-sulfanylidene-1,2,4-triazine-5,6-dione (CCD ID: A1D92) (formula: $C_3H_2N_4O_2S$).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	S	0
			12	3	2	4	2	1	
2	B	1	Total	C	H	N	O	S	0
			12	3	2	4	2	1	

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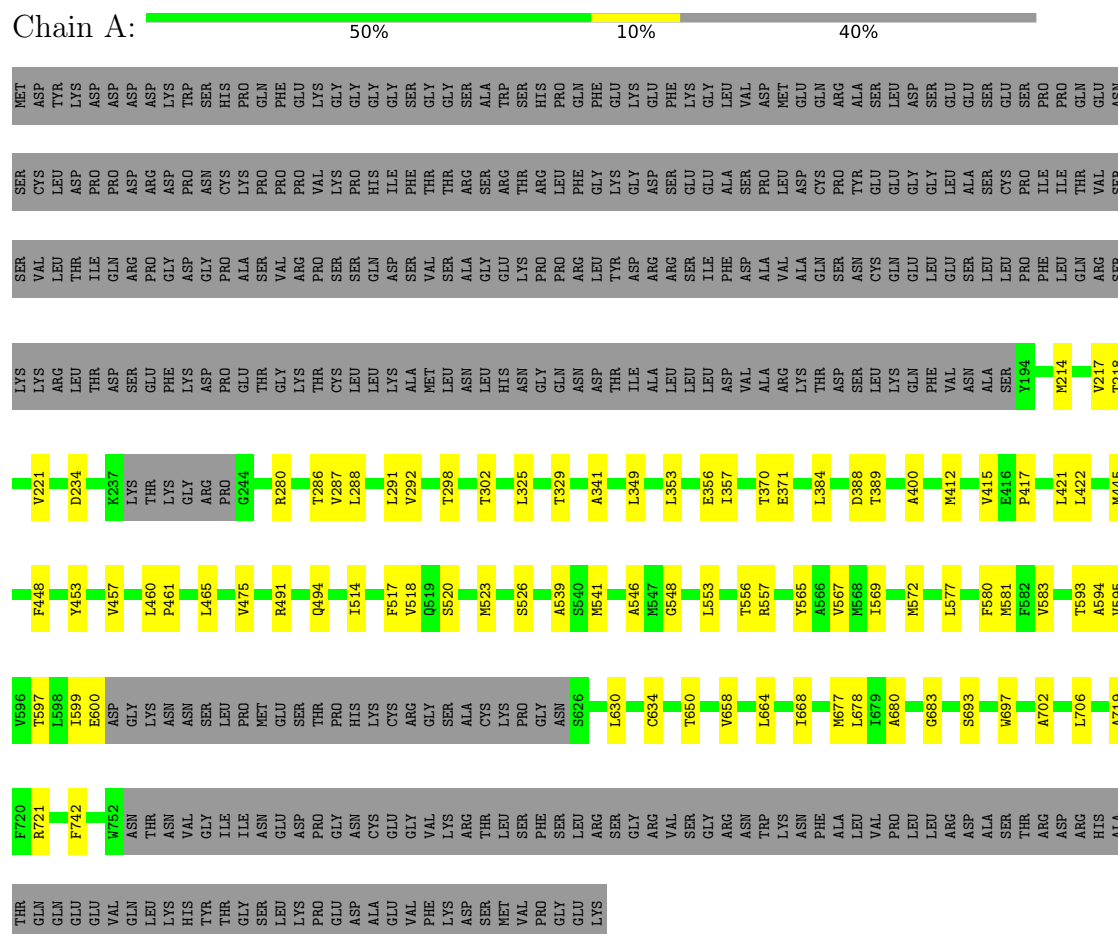
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Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	H	N	O	S	0
			12	3	2	4	2	1	
2	D	1	Total	C	H	N	O	S	0
			12	3	2	4	2	1	

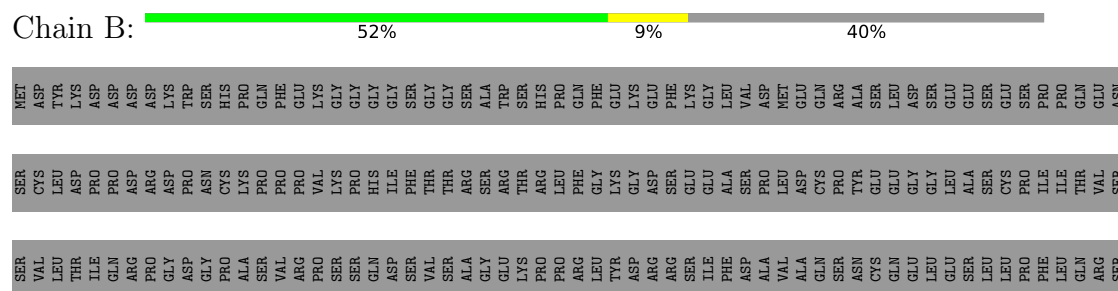
3 Residue-property plots

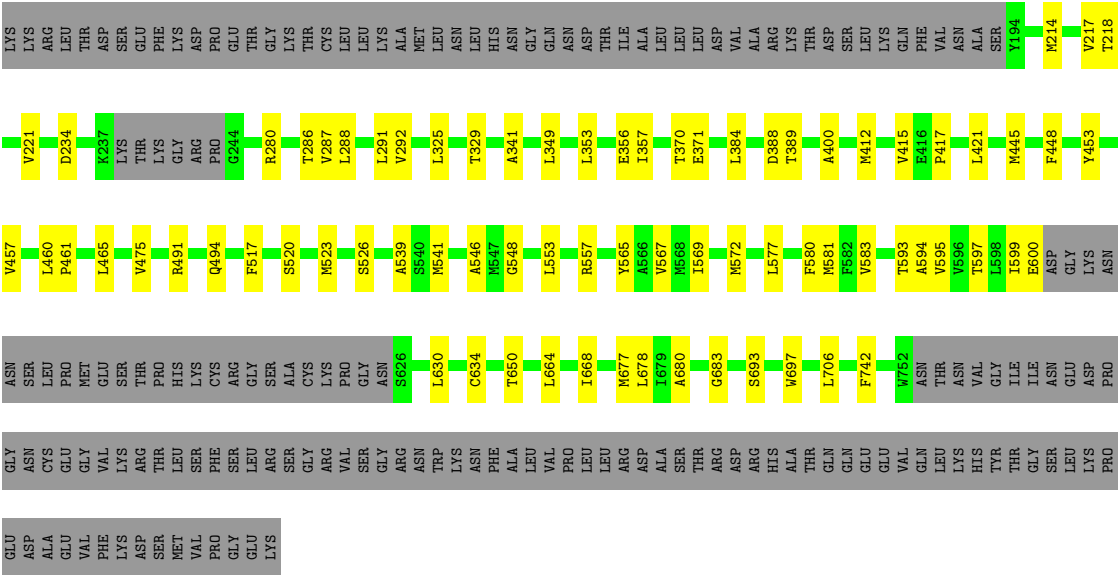
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: Transient receptor potential cation channel subfamily V member 1





● Molecule 1: Transient receptor potential cation channel subfamily V member 1



● Molecule 1: Transient receptor potential cation channel subfamily V member 1



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15808	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (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: A1D92

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	0.10	0/4398	0.27	0/5956
1	B	0.10	0/4398	0.27	0/5956
1	C	0.10	0/4398	0.27	0/5956
1	D	0.10	0/4398	0.27	0/5956
All	All	0.10	0/17592	0.27	0/23824

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	4295	4315	4315	62	0
1	B	4295	4315	4315	56	0
1	C	4295	4315	4315	59	0
1	D	4295	4315	4315	56	0
2	A	10	2	0	0	0
2	B	10	2	0	0	0
2	C	10	2	0	0	0
2	D	10	2	0	0	0
All	All	17220	17268	17260	198	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 (198) 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:B:677:MET:HE1	1:D:569:ILE:HA	1.78	0.66
1:A:677:MET:HE1	1:B:569:ILE:HA	1.78	0.65
1:C:569:ILE:HA	1:D:677:MET:HE1	1.77	0.65
1:A:569:ILE:HA	1:C:677:MET:HE1	1.78	0.65
1:A:353:LEU:HD23	1:A:417:PRO:HG2	1.79	0.64
1:B:353:LEU:HD23	1:B:417:PRO:HG2	1.79	0.64
1:D:353:LEU:HD23	1:D:417:PRO:HG2	1.79	0.64
1:B:341:ALA:O	1:B:412:MET:HE1	1.98	0.64
1:A:341:ALA:O	1:A:412:MET:HE1	1.98	0.63
1:C:353:LEU:HD23	1:C:417:PRO:HG2	1.79	0.63
1:D:341:ALA:O	1:D:412:MET:HE1	1.98	0.63
1:C:341:ALA:O	1:C:412:MET:HE1	1.98	0.62
1:D:214:MET:HE3	1:D:218:THR:HG23	1.82	0.62
1:B:214:MET:HE3	1:B:218:THR:HG23	1.82	0.62
1:A:214:MET:HE3	1:A:218:THR:HG23	1.82	0.61
1:C:214:MET:HE3	1:C:218:THR:HG23	1.82	0.61
1:B:445:MET:HE1	1:B:548:GLY:HA3	1.84	0.60
1:D:445:MET:HE1	1:D:548:GLY:HA3	1.84	0.60
1:A:445:MET:HE1	1:A:548:GLY:HA3	1.84	0.60
1:C:445:MET:HE1	1:C:548:GLY:HA3	1.84	0.60
1:C:572:MET:HG3	1:D:677:MET:HE2	1.86	0.58
1:B:677:MET:HE2	1:D:572:MET:HG3	1.86	0.57
1:B:597:THR:HG22	1:D:453:TYR:HA	1.87	0.57
1:A:677:MET:HE2	1:B:572:MET:HG3	1.86	0.57
1:A:572:MET:HG3	1:C:677:MET:HE2	1.86	0.56
1:C:453:TYR:HA	1:D:597:THR:HG22	1.87	0.56
1:A:453:TYR:HA	1:C:597:THR:HG22	1.86	0.56
1:A:597:THR:HG22	1:B:453:TYR:HA	1.87	0.56
1:B:664:LEU:O	1:B:668:ILE:HG13	2.08	0.53
1:A:593:THR:O	1:A:597:THR:HG23	2.09	0.53
1:D:664:LEU:O	1:D:668:ILE:HG13	2.08	0.53
1:B:593:THR:O	1:B:597:THR:HG23	2.09	0.53
1:C:593:THR:O	1:C:597:THR:HG23	2.09	0.53
1:A:664:LEU:O	1:A:668:ILE:HG13	2.08	0.53
1:B:594:ALA:HB2	1:D:546:ALA:HB2	1.90	0.53
1:C:664:LEU:O	1:C:668:ILE:HG13	2.08	0.53
1:B:599:ILE:CD1	1:B:650:THR:HG21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:ALA:HB2	1:D:594:ALA:HB2	1.90	0.52
1:A:594:ALA:HB2	1:B:546:ALA:HB2	1.90	0.52
1:A:599:ILE:CD1	1:A:650:THR:HG21	2.39	0.52
1:D:593:THR:O	1:D:597:THR:HG23	2.09	0.52
1:A:546:ALA:HB2	1:C:594:ALA:HB2	1.91	0.52
1:C:599:ILE:CD1	1:C:650:THR:HG21	2.39	0.52
1:A:288:LEU:HD11	1:A:325:LEU:HG	1.92	0.52
1:B:288:LEU:HD11	1:B:325:LEU:HG	1.92	0.51
1:D:599:ILE:CD1	1:D:650:THR:HG21	2.39	0.51
1:C:288:LEU:HD11	1:C:325:LEU:HG	1.92	0.51
1:A:400:ALA:HB3	1:A:706:LEU:HD12	1.93	0.51
1:B:599:ILE:HD11	1:B:650:THR:HG21	1.92	0.51
1:D:288:LEU:HD11	1:D:325:LEU:HG	1.92	0.51
1:C:400:ALA:HB3	1:C:706:LEU:HD12	1.93	0.51
1:C:553:LEU:HD21	1:D:583:VAL:HG22	1.93	0.51
1:D:595:VAL:HG12	1:D:599:ILE:HD12	1.92	0.51
1:B:356:GLU:OE1	1:B:357:ILE:N	2.44	0.50
1:B:400:ALA:HB3	1:B:706:LEU:HD12	1.93	0.50
1:B:595:VAL:HG12	1:B:599:ILE:HD12	1.92	0.50
1:C:356:GLU:OE1	1:C:357:ILE:N	2.44	0.50
1:A:595:VAL:HG12	1:A:599:ILE:HD12	1.92	0.50
1:D:356:GLU:OE1	1:D:357:ILE:N	2.44	0.50
1:D:599:ILE:HD11	1:D:650:THR:HG21	1.92	0.50
1:A:356:GLU:OE1	1:A:357:ILE:N	2.44	0.50
1:A:599:ILE:HD11	1:A:650:THR:HG21	1.92	0.50
1:B:583:VAL:HG22	1:D:553:LEU:HD21	1.93	0.50
1:A:553:LEU:HD21	1:C:583:VAL:HG22	1.93	0.49
1:A:583:VAL:HG22	1:B:553:LEU:HD21	1.93	0.49
1:B:389:THR:O	1:B:389:THR:HG23	2.12	0.49
1:A:389:THR:O	1:A:389:THR:HG23	2.13	0.49
1:D:400:ALA:HB3	1:D:706:LEU:HD12	1.93	0.49
1:C:517:PHE:O	1:C:520:SER:OG	2.28	0.49
1:C:557:ARG:O	1:C:697:TRP:NE1	2.44	0.49
1:C:595:VAL:HG12	1:C:599:ILE:HD12	1.92	0.49
1:A:557:ARG:O	1:A:697:TRP:NE1	2.44	0.49
1:C:388:ASP:OD1	1:C:389:THR:N	2.45	0.49
1:C:599:ILE:HD11	1:C:650:THR:HG21	1.92	0.49
1:D:388:ASP:OD1	1:D:389:THR:N	2.45	0.49
1:C:389:THR:HG23	1:C:389:THR:O	2.12	0.49
1:D:389:THR:HG23	1:D:389:THR:O	2.12	0.48
1:C:448:PHE:CZ	1:C:523:MET:HE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:ARG:O	1:D:697:TRP:NE1	2.44	0.47
1:B:491:ARG:NH1	1:B:494:GLN:OE1	2.48	0.47
1:A:448:PHE:CZ	1:A:523:MET:HE1	2.49	0.47
1:B:217:VAL:O	1:B:221:VAL:HG23	2.15	0.47
1:B:388:ASP:OD1	1:B:389:THR:N	2.45	0.47
1:C:217:VAL:O	1:C:221:VAL:HG23	2.15	0.47
1:D:491:ARG:NH1	1:D:494:GLN:OE1	2.48	0.47
1:A:217:VAL:O	1:A:221:VAL:HG23	2.15	0.47
1:A:491:ARG:NH1	1:A:494:GLN:OE1	2.48	0.47
1:D:448:PHE:CZ	1:D:523:MET:HE1	2.50	0.47
1:C:491:ARG:NH1	1:C:494:GLN:OE1	2.48	0.47
1:D:217:VAL:O	1:D:221:VAL:HG23	2.15	0.46
1:B:448:PHE:CZ	1:B:523:MET:HE1	2.50	0.46
1:A:388:ASP:OD1	1:A:389:THR:N	2.45	0.46
1:A:517:PHE:O	1:A:520:SER:OG	2.28	0.46
1:A:577:LEU:HD23	1:A:581:MET:HG2	1.98	0.46
1:B:280:ARG:NH1	1:B:329:THR:O	2.49	0.46
1:B:567:VAL:HG11	1:B:693:SER:HA	1.98	0.46
1:D:567:VAL:HG11	1:D:693:SER:HA	1.98	0.46
1:A:567:VAL:HG11	1:A:693:SER:HA	1.98	0.45
1:C:567:VAL:HG11	1:C:693:SER:HA	1.98	0.45
1:A:280:ARG:NH1	1:A:329:THR:O	2.49	0.45
1:B:577:LEU:HD23	1:B:581:MET:HG2	1.98	0.45
1:D:280:ARG:NH1	1:D:329:THR:O	2.49	0.45
1:A:298:THR:O	1:A:302:THR:N	2.42	0.45
1:D:577:LEU:HD23	1:D:581:MET:HG2	1.98	0.45
1:A:553:LEU:O	1:A:556:THR:OG1	2.27	0.45
1:B:557:ARG:O	1:B:697:TRP:NE1	2.44	0.45
1:B:384:LEU:HD13	1:B:421:LEU:HD11	2.00	0.44
1:C:577:LEU:HD23	1:C:581:MET:HG2	1.98	0.44
1:B:517:PHE:O	1:B:520:SER:OG	2.28	0.44
1:C:280:ARG:NH1	1:C:329:THR:O	2.49	0.44
1:C:384:LEU:HD13	1:C:421:LEU:HD11	2.00	0.44
1:C:460:LEU:O	1:C:461:PRO:C	2.61	0.44
1:D:460:LEU:O	1:D:461:PRO:C	2.61	0.44
1:C:298:THR:O	1:C:302:THR:N	2.42	0.44
1:B:288:LEU:O	1:B:292:VAL:HG23	2.18	0.44
1:D:288:LEU:O	1:D:292:VAL:HG23	2.18	0.44
1:A:288:LEU:O	1:A:292:VAL:HG23	2.18	0.44
1:B:415:VAL:HG12	1:B:417:PRO:HD2	2.00	0.44
1:A:415:VAL:HG12	1:A:417:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LEU:HD13	1:B:475:VAL:HG21	2.01	0.43
1:A:460:LEU:O	1:A:461:PRO:C	2.61	0.43
1:B:460:LEU:O	1:B:461:PRO:C	2.61	0.43
1:C:565:TYR:CE2	1:D:583:VAL:HG21	2.53	0.43
1:A:457:VAL:HG12	1:A:457:VAL:O	2.18	0.43
1:B:583:VAL:HG21	1:D:565:TYR:CE2	2.53	0.43
1:A:384:LEU:HD13	1:A:421:LEU:HD11	2.00	0.43
1:A:583:VAL:HG21	1:B:565:TYR:CE2	2.53	0.43
1:A:465:LEU:HD13	1:A:475:VAL:HG21	2.01	0.43
1:A:565:TYR:CE2	1:C:583:VAL:HG21	2.54	0.43
1:D:465:LEU:HD13	1:D:475:VAL:HG21	2.01	0.43
1:B:286:THR:HG23	1:B:287:VAL:N	2.34	0.43
1:D:384:LEU:HD13	1:D:421:LEU:HD11	2.00	0.43
1:D:457:VAL:HG12	1:D:457:VAL:O	2.18	0.43
1:D:370:THR:HG22	1:D:371:GLU:N	2.34	0.43
1:B:349:LEU:HD22	1:B:412:MET:SD	2.59	0.43
1:C:286:THR:HG23	1:C:287:VAL:N	2.34	0.43
1:C:457:VAL:O	1:C:457:VAL:HG12	2.18	0.43
1:D:415:VAL:HG12	1:D:417:PRO:HD2	2.00	0.43
1:A:349:LEU:HD22	1:A:412:MET:SD	2.59	0.42
1:B:370:THR:HG22	1:B:371:GLU:N	2.34	0.42
1:B:457:VAL:HG12	1:B:457:VAL:O	2.18	0.42
1:C:465:LEU:HD13	1:C:475:VAL:HG21	2.01	0.42
1:C:349:LEU:HD22	1:C:412:MET:SD	2.59	0.42
1:D:287:VAL:O	1:D:291:LEU:HD23	2.20	0.42
1:A:287:VAL:O	1:A:291:LEU:HD23	2.20	0.42
1:B:680:ALA:HB1	1:D:683:GLY:HA2	2.01	0.42
1:C:288:LEU:O	1:C:292:VAL:HG23	2.18	0.42
1:C:678:LEU:O	1:C:678:LEU:HD12	2.20	0.42
1:D:286:THR:HG23	1:D:287:VAL:N	2.34	0.42
1:D:384:LEU:HD11	1:D:742:PHE:HB2	2.02	0.42
1:B:287:VAL:O	1:B:291:LEU:HD23	2.20	0.42
1:B:678:LEU:HD12	1:B:678:LEU:O	2.20	0.42
1:C:683:GLY:HA2	1:D:680:ALA:HB1	2.01	0.42
1:A:630:LEU:HD23	1:A:634:CYS:SG	2.60	0.42
1:C:370:THR:HG22	1:C:371:GLU:N	2.34	0.42
1:C:415:VAL:HG12	1:C:417:PRO:HD2	2.00	0.42
1:D:349:LEU:HD22	1:D:412:MET:SD	2.59	0.42
1:A:594:ALA:CB	1:B:546:ALA:HB2	2.50	0.42
1:A:683:GLY:HA2	1:C:680:ALA:HB1	2.02	0.42
1:B:580:PHE:CG	1:B:678:LEU:HD22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:HD11	1:A:742:PHE:HB2	2.02	0.42
1:A:678:LEU:HD12	1:A:678:LEU:O	2.20	0.42
1:D:630:LEU:HD23	1:D:634:CYS:SG	2.60	0.42
1:D:678:LEU:HD12	1:D:678:LEU:O	2.20	0.42
1:A:370:THR:HG22	1:A:371:GLU:N	2.34	0.42
1:A:680:ALA:HB1	1:B:683:GLY:HA2	2.01	0.42
1:B:630:LEU:HD23	1:B:634:CYS:SG	2.60	0.42
1:B:594:ALA:CB	1:D:546:ALA:HB2	2.50	0.41
1:D:234:ASP:OD1	1:D:234:ASP:N	2.53	0.41
1:A:580:PHE:CG	1:A:678:LEU:HD22	2.55	0.41
1:A:286:THR:HG23	1:A:287:VAL:N	2.34	0.41
1:C:546:ALA:HB2	1:D:594:ALA:CB	2.50	0.41
1:C:630:LEU:HD23	1:C:634:CYS:SG	2.60	0.41
1:A:526:SER:OG	1:A:541:MET:N	2.54	0.41
1:C:580:PHE:CG	1:C:678:LEU:HD22	2.55	0.41
1:D:580:PHE:CG	1:D:678:LEU:HD22	2.55	0.41
1:A:546:ALA:HB2	1:C:594:ALA:CB	2.51	0.41
1:C:384:LEU:HD11	1:C:742:PHE:HB2	2.02	0.41
1:C:526:SER:OG	1:C:541:MET:N	2.54	0.41
1:C:287:VAL:O	1:C:291:LEU:HD23	2.20	0.41
1:A:599:ILE:O	1:A:600:GLU:CB	2.69	0.41
1:B:234:ASP:OD1	1:B:234:ASP:N	2.53	0.41
1:B:526:SER:OG	1:B:541:MET:N	2.54	0.41
1:C:422:LEU:HD13	1:C:702:ALA:HB2	2.03	0.41
1:C:539:ALA:HB1	1:D:658:VAL:HG21	2.03	0.41
1:B:384:LEU:HD11	1:B:742:PHE:HB2	2.02	0.41
1:A:514:ILE:O	1:A:518:VAL:HG23	2.21	0.40
1:D:517:PHE:O	1:D:520:SER:OG	2.28	0.40
1:A:422:LEU:HD13	1:A:702:ALA:HB2	2.02	0.40
1:A:719:ALA:O	1:A:721:ARG:NH1	2.55	0.40
1:C:234:ASP:OD1	1:C:234:ASP:N	2.53	0.40
1:C:719:ALA:O	1:C:721:ARG:NH1	2.55	0.40
1:D:514:ILE:O	1:D:518:VAL:HG23	2.21	0.40
1:A:539:ALA:HB1	1:C:658:VAL:HG21	2.03	0.40
1:B:599:ILE:O	1:B:600:GLU:CB	2.69	0.40
1:D:599:ILE:O	1:D:600:GLU:CB	2.69	0.40
1:A:234:ASP:N	1:A:234:ASP:OD1	2.53	0.40
1:A:658:VAL:HG21	1:B:539:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	522/879 (59%)	493 (94%)	29 (6%)	0	100	100
1	B	522/879 (59%)	493 (94%)	29 (6%)	0	100	100
1	C	522/879 (59%)	493 (94%)	29 (6%)	0	100	100
1	D	522/879 (59%)	493 (94%)	29 (6%)	0	100	100
All	All	2088/3516 (59%)	1972 (94%)	116 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	468/775 (60%)	468 (100%)	0	100	100
1	B	468/775 (60%)	468 (100%)	0	100	100
1	C	468/775 (60%)	468 (100%)	0	100	100
1	D	468/775 (60%)	468 (100%)	0	100	100
All	All	1872/3100 (60%)	1872 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	354	GLN
1	B	232	ASN
1	B	354	GLN
1	C	232	ASN
1	C	354	GLN
1	D	232	ASN
1	D	354	GLN

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 oligosaccharides 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	A1D92	A	901	-	9,10,10	4.08	7 (77%)	5,14,14	2.91	2 (40%)
2	A1D92	B	901	-	9,10,10	4.08	7 (77%)	5,14,14	2.91	2 (40%)
2	A1D92	D	901	-	9,10,10	4.09	6 (66%)	5,14,14	2.90	2 (40%)
2	A1D92	C	901	-	9,10,10	4.08	7 (77%)	5,14,14	2.91	2 (40%)

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	A1D92	A	901	-	-	-	0/1/1/1
2	A1D92	B	901	-	-	-	0/1/1/1
2	A1D92	D	901	-	-	-	0/1/1/1
2	A1D92	C	901	-	-	-	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	A1D92	C01-N09	9.20	1.48	1.35
2	B	901	A1D92	C01-N09	9.20	1.48	1.35
2	C	901	A1D92	C01-N09	9.20	1.48	1.35
2	D	901	A1D92	C01-N09	9.20	1.48	1.35
2	A	901	A1D92	N09-N08	4.88	1.43	1.31
2	B	901	A1D92	N09-N08	4.88	1.43	1.31
2	C	901	A1D92	N09-N08	4.88	1.43	1.31
2	D	901	A1D92	N09-N08	4.88	1.43	1.31
2	D	901	A1D92	C06-N08	3.41	1.45	1.38
2	A	901	A1D92	C06-N08	3.37	1.44	1.38
2	B	901	A1D92	C06-N08	3.37	1.44	1.38
2	C	901	A1D92	C06-N08	3.37	1.44	1.38
2	C	901	A1D92	C01-S02	-3.14	1.59	1.67
2	A	901	A1D92	C01-S02	-3.14	1.59	1.67
2	B	901	A1D92	C01-S02	-3.14	1.59	1.67
2	D	901	A1D92	C01-S02	-3.14	1.59	1.67
2	A	901	A1D92	O07-C06	-3.06	1.18	1.23
2	B	901	A1D92	O07-C06	-3.06	1.18	1.23
2	C	901	A1D92	O07-C06	-3.06	1.18	1.23
2	D	901	A1D92	O07-C06	-3.06	1.18	1.23
2	A	901	A1D92	C04-N03	2.42	1.43	1.39
2	B	901	A1D92	C04-N03	2.42	1.43	1.39
2	C	901	A1D92	C04-N03	2.42	1.43	1.39
2	D	901	A1D92	C04-N03	2.42	1.43	1.39
2	A	901	A1D92	O05-C04	-2.00	1.18	1.23
2	B	901	A1D92	O05-C04	-2.00	1.18	1.23
2	C	901	A1D92	O05-C04	-2.00	1.18	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	A1D92	C06-C04-N03	5.85	119.92	117.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	A1D92	C06-C04-N03	5.85	119.92	117.84
2	C	901	A1D92	C06-C04-N03	5.85	119.92	117.84
2	D	901	A1D92	C06-C04-N03	5.85	119.92	117.84
2	A	901	A1D92	C06-N08-N09	2.34	120.00	118.06
2	B	901	A1D92	C06-N08-N09	2.34	120.00	118.06
2	C	901	A1D92	C06-N08-N09	2.34	120.00	118.06
2	D	901	A1D92	C06-N08-N09	2.31	119.98	118.06

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.