Full wwPDB EM Validation Report

Jun 1, 2025 – 12:07 AM JST

PDB ID	:	9L3Z / pdb_00009l3z
EMDB ID	:	EMD-62799
Title	:	Cryo-EM structure of the inactive chemokine-like receptor 1 (CMKLR1)
Authors	:	Zhu, Y.; He, M.; Wu, B.; Zhao, Q.
Deposited on	:	2024-12-19
Resolution	:	3.90 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:

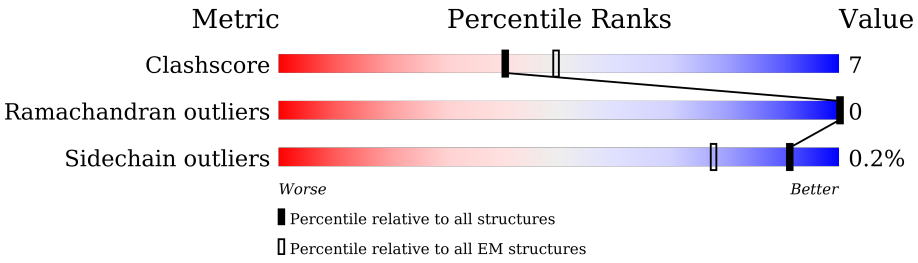
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.90 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%

Mol	Chain	Length	Quality of chain
1	H	252	63% 17% 19%
2	L	216	68% 16% 16%
3	A	498	63% 6% 30%
4	C	7	29% 71%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5147 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 The heavy chain of anti-BRIL Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	203	Total	C	N	O	S	0	0
			1531	982	251	293	5		

- Molecule 2 is a protein called The light chain of anti-BRIL Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	181	Total	C	N	O	S	0	0
			1379	870	222	282	5		

- Molecule 3 is a protein called Chemerin-like receptor 1,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	348	Total	C	N	O	S	0	0
			2213	1373	402	429	9		

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ALA	-	linker	UNP Q99788
A	252	ARG	-	linker	UNP Q99788
A	253	ARG	-	linker	UNP Q99788
A	254	GLN	-	linker	UNP Q99788
A	255	LEU	-	linker	UNP Q99788
A	262	TRP	MET	conflict	UNP P0ABE7
A	357	ILE	HIS	conflict	UNP P0ABE7
A	361	LEU	-	linker	UNP P0ABE7
A	362	GLU	-	linker	UNP P0ABE7
A	363	ARG	-	linker	UNP P0ABE7
A	364	ALA	-	linker	UNP P0ABE7
A	365	ARG	-	linker	UNP P0ABE7
A	366	SER	-	linker	UNP P0ABE7
A	?	THR	-	linker	UNP P0ABE7
A	?	LEU	-	linker	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	373	ASP	PHE	engineered mutation	UNP Q99788
A	453	GLU	-	expression tag	UNP Q99788
A	454	PHE	-	expression tag	UNP Q99788
A	455	LEU	-	expression tag	UNP Q99788
A	456	GLU	-	expression tag	UNP Q99788
A	457	VAL	-	expression tag	UNP Q99788
A	458	LEU	-	expression tag	UNP Q99788
A	459	PHE	-	expression tag	UNP Q99788
A	460	GLN	-	expression tag	UNP Q99788
A	461	GLY	-	expression tag	UNP Q99788
A	462	PRO	-	expression tag	UNP Q99788
A	463	TRP	-	expression tag	UNP Q99788
A	464	SER	-	expression tag	UNP Q99788
A	465	HIS	-	expression tag	UNP Q99788
A	466	PRO	-	expression tag	UNP Q99788
A	467	GLN	-	expression tag	UNP Q99788
A	468	PHE	-	expression tag	UNP Q99788
A	469	GLU	-	expression tag	UNP Q99788
A	470	LYS	-	expression tag	UNP Q99788
A	471	GLY	-	expression tag	UNP Q99788
A	472	GLY	-	expression tag	UNP Q99788
A	473	GLY	-	expression tag	UNP Q99788
A	474	SER	-	expression tag	UNP Q99788
A	475	GLY	-	expression tag	UNP Q99788
A	476	GLY	-	expression tag	UNP Q99788
A	477	GLY	-	expression tag	UNP Q99788
A	478	SER	-	expression tag	UNP Q99788
A	479	GLY	-	expression tag	UNP Q99788
A	480	GLY	-	expression tag	UNP Q99788
A	481	SER	-	expression tag	UNP Q99788
A	482	ALA	-	expression tag	UNP Q99788
A	483	TRP	-	expression tag	UNP Q99788
A	484	SER	-	expression tag	UNP Q99788
A	485	HIS	-	expression tag	UNP Q99788
A	486	PRO	-	expression tag	UNP Q99788
A	487	GLN	-	expression tag	UNP Q99788
A	488	PHE	-	expression tag	UNP Q99788
A	489	GLU	-	expression tag	UNP Q99788
A	490	LYS	-	expression tag	UNP Q99788
A	491	ASP	-	expression tag	UNP Q99788
A	492	TYR	-	expression tag	UNP Q99788
A	493	LYS	-	expression tag	UNP Q99788

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Chain	Residue	Modelled	Actual	Comment	Reference
A	494	ASP	-	expression tag	UNP Q99788
A	495	ASP	-	expression tag	UNP Q99788
A	496	ASP	-	expression tag	UNP Q99788
A	497	ASP	-	expression tag	UNP Q99788
A	498	LYS	-	expression tag	UNP Q99788

- Molecule 4 is a protein called LRH7-C2.

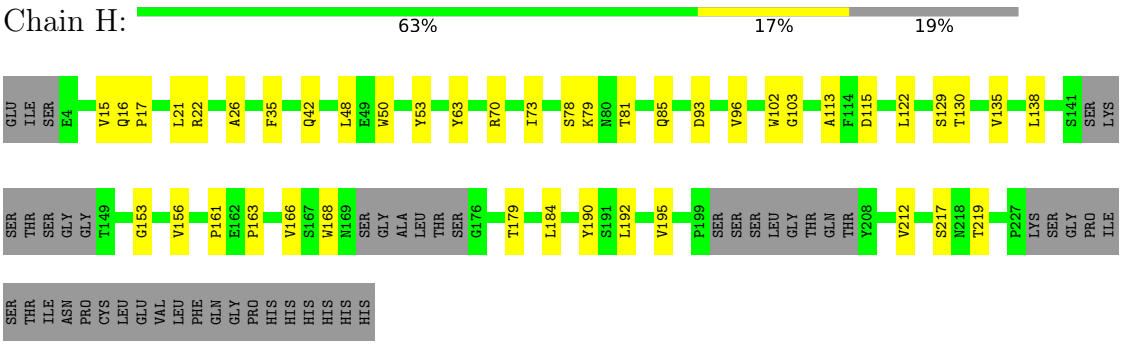
Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	2	Total	C	N	O	0	0
			24	17	5	2		

3 Residue-property plots (i)

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.

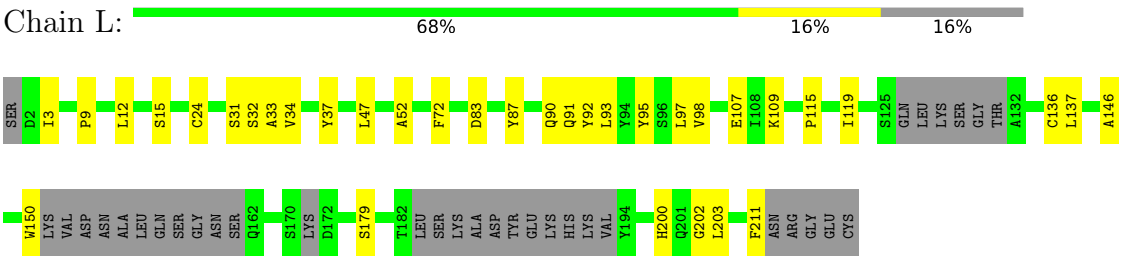
• Molecule 1: The heavy chain of anti-BRIL Fab

Chain H:



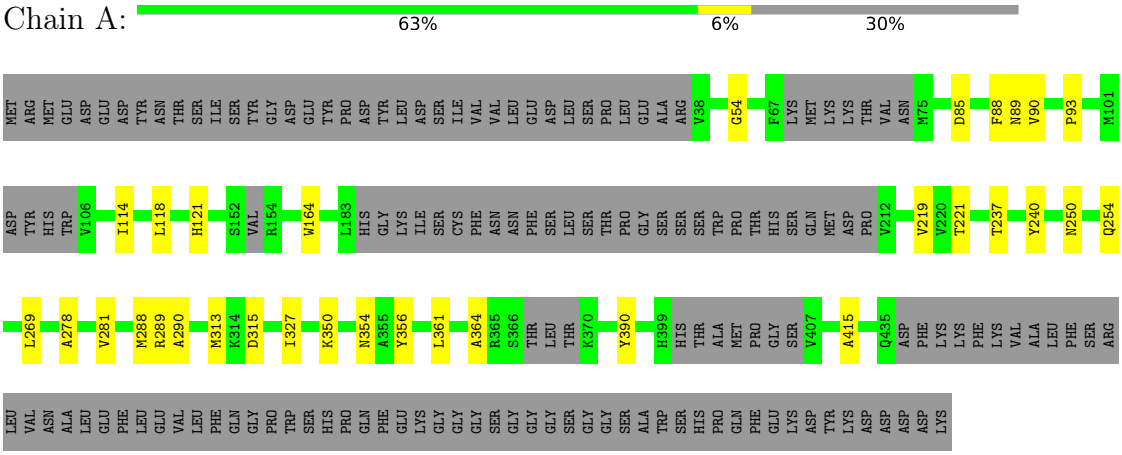
• Molecule 2: The light chain of anti-BRIL Fab

Chain L:



• Molecule 3: Chemerin-like receptor 1,Soluble cytochrome b562

Chain A:



• Molecule 4: LRH7-C2

Chain C:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	260967	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	H	0.14	0/1576	0.28	0/2157
2	L	0.11	0/1408	0.28	0/1917
3	A	0.15	0/2236	0.35	0/3066
4	C	0.06	0/10	0.08	0/12
All	All	0.14	0/5230	0.31	0/7152

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

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	H	1531	0	1449	28	0
2	L	1379	0	1309	25	0
3	A	2213	0	1731	18	0
4	C	24	0	19	1	0
All	All	5147	0	4508	66	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 7.

All (66) 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)
4:C:1:HIS:O	4:C:2:DTR:C	2.42	0.68
2:L:93:LEU:HD21	3:A:290:ALA:HB2	1.77	0.66
3:A:350:LYS:O	3:A:354:ASN:ND2	2.31	0.64
2:L:83:ASP:OD1	2:L:87:TYR:OH	2.17	0.62
2:L:136:CYS:HB3	2:L:179:SER:HB3	1.82	0.62
3:A:315:ASP:OD1	3:A:356:TYR:OH	2.12	0.62
2:L:9:PRO:HB2	2:L:12:LEU:HD21	1.83	0.59
1:H:115:ASP:OD1	1:H:115:ASP:N	2.36	0.58
1:H:70:ARG:NH2	1:H:93:ASP:OD2	2.37	0.58
3:A:250:ASN:O	3:A:254:GLN:HG2	2.05	0.55
3:A:114:ILE:HA	3:A:118:LEU:HD12	1.90	0.54
2:L:34:VAL:HG22	2:L:52:ALA:HB2	1.88	0.53
2:L:24:CYS:O	2:L:72:PHE:N	2.41	0.53
2:L:200:HIS:CD2	2:L:202:GLY:H	2.27	0.53
2:L:91:GLN:NE2	2:L:97:LEU:O	2.41	0.52
2:L:90:GLN:HE21	2:L:98:VAL:HG13	1.75	0.52
1:H:135:VAL:HG22	1:H:156:VAL:HG12	1.91	0.51
3:A:114:ILE:HG23	3:A:118:LEU:HD12	1.92	0.51
3:A:88:PHE:HB2	3:A:118:LEU:HB3	1.91	0.51
2:L:115:PRO:HD2	2:L:203:LEU:HG	1.92	0.51
2:L:31:SER:OG	2:L:32:SER:N	2.44	0.50
3:A:278:ALA:HA	3:A:281:VAL:HG12	1.93	0.49
3:A:121:HIS:HE2	3:A:164:TRP:CD1	2.31	0.49
1:H:195:VAL:HG11	2:L:137:LEU:HD21	1.95	0.48
1:H:22:ARG:NH1	1:H:85:GLN:OE1	2.44	0.48
3:A:361:LEU:HA	3:A:364:ALA:HB3	1.96	0.47
1:H:179:THR:HG23	1:H:192:LEU:HD21	1.97	0.47
1:H:50:TRP:HZ2	1:H:53:TYR:HB3	1.79	0.47
1:H:103:GLY:O	2:L:95:TYR:OH	2.23	0.47
2:L:37:TYR:HD1	2:L:47:LEU:HA	1.80	0.47
1:H:15:VAL:HG21	1:H:21:LEU:HD22	1.96	0.46
3:A:289:ARG:HB2	3:A:327:ILE:HG21	1.96	0.46
2:L:119:ILE:HD11	2:L:211:PHE:HD1	1.81	0.46
1:H:166:VAL:HG12	1:H:212:VAL:HG12	1.99	0.45
2:L:146:ALA:HB2	2:L:200:HIS:ND1	2.32	0.45
2:L:31:SER:O	2:L:33:ALA:N	2.50	0.45
2:L:12:LEU:O	2:L:107:GLU:HG2	2.17	0.45
1:H:78:SER:OG	1:H:79:LYS:NZ	2.50	0.45
3:A:54:GLY:HA3	3:A:89:ASN:HD21	1.82	0.44
1:H:153:GLY:HA2	1:H:168:TRP:HZ2	1.83	0.44
2:L:3:ILE:HD11	2:L:91:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:PRO:HG2	1:H:163:PRO:HD2	1.99	0.43
1:H:16:GLN:HG2	1:H:17:PRO:HD2	2.00	0.43
3:A:219:VAL:O	3:A:221:THR:HG23	2.19	0.43
3:A:237:THR:HA	3:A:240:TYR:CE2	2.54	0.43
1:H:113:ALA:HB2	2:L:92:TYR:CE1	2.54	0.42
3:A:390:TYR:HE1	3:A:415:ALA:HB1	1.84	0.42
1:H:153:GLY:HA2	1:H:168:TRP:CZ2	2.55	0.42
2:L:15:SER:HB2	2:L:109:LYS:HB3	2.00	0.42
1:H:63:TYR:HE1	1:H:73:ILE:HG22	1.85	0.41
1:H:42:GLN:HB2	1:H:48:LEU:HD23	2.02	0.41
1:H:138:LEU:HB3	1:H:153:GLY:O	2.20	0.41
3:A:90:VAL:O	3:A:93:PRO:HD2	2.21	0.41
1:H:35:PHE:CD1	1:H:103:GLY:HA2	2.55	0.41
1:H:102:TRP:CH2	2:L:92:TYR:HB2	2.56	0.41
3:A:85:ASP:HA	3:A:88:PHE:CE1	2.56	0.41
1:H:96:VAL:HA	1:H:122:LEU:HA	2.03	0.41
1:H:184:LEU:HD12	1:H:190:TYR:HE1	1.86	0.41
1:H:26:ALA:HA	1:H:81:THR:HG22	2.02	0.41
1:H:129:SER:OG	1:H:130:THR:N	2.54	0.40
3:A:269:LEU:HD13	3:A:288:MET:HE1	2.02	0.40
2:L:150:TRP:NE1	2:L:179:SER:OG	2.40	0.40
1:H:53:TYR:CE2	2:L:95:TYR:HD2	2.40	0.40
2:L:203:LEU:HD23	2:L:203:LEU:HA	1.90	0.40
1:H:217:SER:O	1:H:219:THR:HG23	2.21	0.40
1:H:35:PHE:HD1	1:H:103:GLY:HA2	1.86	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	H	195/252 (77%)	186 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	171/216 (79%)	160 (94%)	11 (6%)	0	100	100
3	A	334/498 (67%)	311 (93%)	23 (7%)	0	100	100
All	All	700/966 (72%)	657 (94%)	43 (6%)	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	H	165/211 (78%)	165 (100%)	0	100	100
2	L	158/191 (83%)	158 (100%)	0	100	100
3	A	149/435 (34%)	148 (99%)	1 (1%)	81	86
4	C	1/6 (17%)	1 (100%)	0	100	100
All	All	473/843 (56%)	472 (100%)	1 (0%)	91	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	313	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	162	GLN
2	L	168	GLN
3	A	296	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
4	DTR	C	2	4	13,15,16	0.69	0	13,20,22	0.83	0

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
4	DTR	C	2	4	-	0/4/6/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2	DTR	1	0

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.