



Full wwPDB EM Validation Report ⓘ

Nov 10, 2025 – 04:17 PM JST

PDB ID : 9X1H / pdb_00009x1h
EMDB ID : EMD-66460
Title : Cryo-EM Structure of human complement C1s CUB domain in complex with RAY121
Authors : Kawauchi, H.; Adrian, H.; Gupta, G.; Koga, H.; Fujii, T.; Fukumura, T.; Ishino, S.; Irie, M.; Torizawa, T.
Deposited on : 2025-10-02
Resolution : 2.60 Å (reported)
Based on initial models : ., 4LMF

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB 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:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

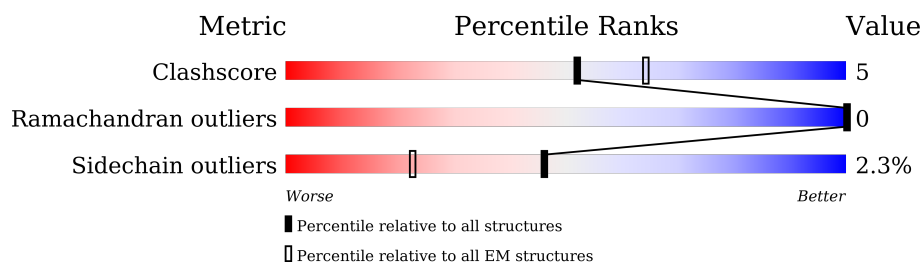
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	L	220	43% 7% 50%
1	M	220	43% 7% 50%
2	H	225	40% 10% 50%
2	I	225	39% 11% 50%
3	A	290	48% . 47%
3	B	290	48% 5% . 47%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5888 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 RAY121 Fab Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	110	Total	C	N	O	S	0	0
			838	525	142	168	3		
1	M	110	Total	C	N	O	S	0	0
			838	525	142	168	3		

- Molecule 2 is a protein called RAY121 Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	113	Total	C	N	O	S	0	0
			871	556	150	162	3		
2	H	113	Total	C	N	O	S	0	0
			871	556	150	162	3		

- Molecule 3 is a protein called Complement C1s subcomponent heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	154	Total	C	N	O	S	0	0
			1233	781	194	248	10		
3	A	154	Total	C	N	O	S	0	0
			1233	781	194	248	10		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	278	GLY	-	expression tag	UNP P09871
B	279	GLY	-	expression tag	UNP P09871
B	280	GLY	-	expression tag	UNP P09871
B	281	GLY	-	expression tag	UNP P09871
B	282	SER	-	expression tag	UNP P09871
B	283	ASP	-	expression tag	UNP P09871
B	284	TYR	-	expression tag	UNP P09871
B	285	LYS	-	expression tag	UNP P09871
B	286	ASP	-	expression tag	UNP P09871

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Chain	Residue	Modelled	Actual	Comment	Reference
B	287	ASP	-	expression tag	UNP P09871
B	288	ASP	-	expression tag	UNP P09871
B	289	ASP	-	expression tag	UNP P09871
B	290	LYS	-	expression tag	UNP P09871
A	278	GLY	-	expression tag	UNP P09871
A	279	GLY	-	expression tag	UNP P09871
A	280	GLY	-	expression tag	UNP P09871
A	281	GLY	-	expression tag	UNP P09871
A	282	SER	-	expression tag	UNP P09871
A	283	ASP	-	expression tag	UNP P09871
A	284	TYR	-	expression tag	UNP P09871
A	285	LYS	-	expression tag	UNP P09871
A	286	ASP	-	expression tag	UNP P09871
A	287	ASP	-	expression tag	UNP P09871
A	288	ASP	-	expression tag	UNP P09871
A	289	ASP	-	expression tag	UNP P09871
A	290	LYS	-	expression tag	UNP P09871

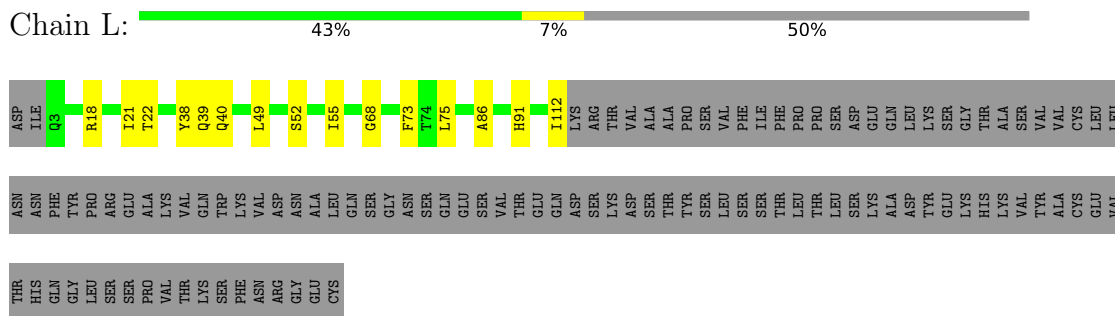
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	B	2	Total Ca 2 2	0
4	A	2	Total Ca 2 2	0

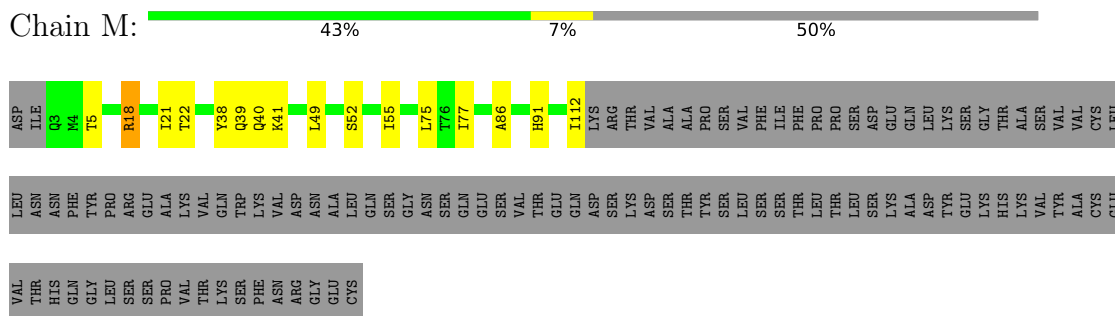
3 Residue-property plots

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.

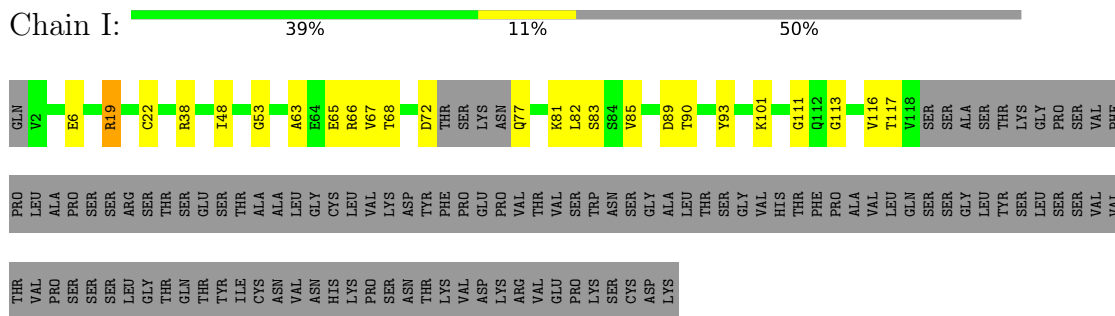
- Molecule 1: RAY121 Fab Light chain



- Molecule 1: RAY121 Fab Light chain

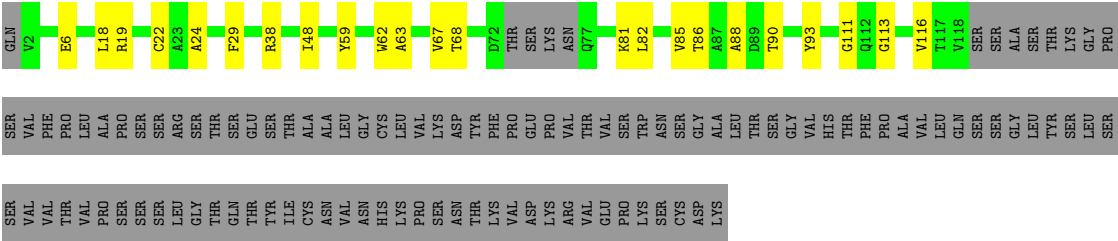


- Molecule 2: RAY121 Fab Heavy chain

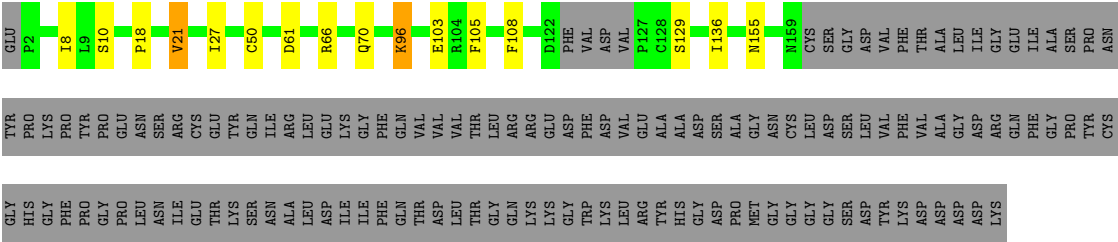


- Molecule 2: RAY121 Fab Heavy chain

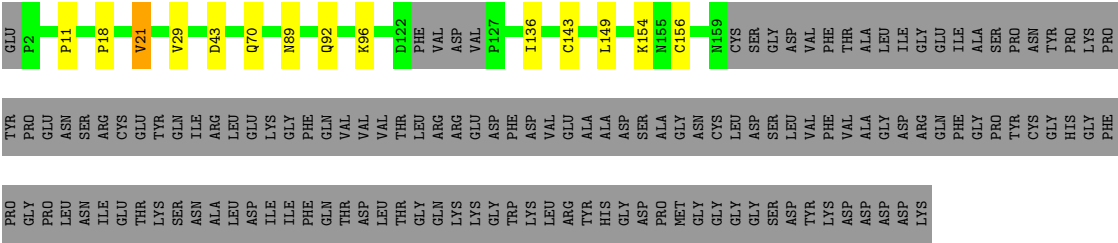




• Molecule 3: Complement C1s subcomponent heavy chain



• Molecule 3: Complement C1s subcomponent heavy chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1101481	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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: CA

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	L	0.15	0/859	0.42	0/1164
1	M	0.15	0/859	0.39	0/1164
2	H	0.17	0/893	0.41	0/1211
2	I	0.15	0/893	0.41	0/1211
3	A	0.15	0/1270	0.36	0/1726
3	B	0.16	0/1270	0.39	0/1726
All	All	0.15	0/6044	0.39	0/8202

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	L	838	0	796	6	0
1	M	838	0	796	7	0
2	H	871	0	837	16	0
2	I	871	0	837	15	0
3	A	1233	0	1107	9	0
3	B	1233	0	1107	8	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
All	All	5888	0	5480	59	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 5.

All (59) 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)
2:I:53:GLY:HA3	2:I:101:LYS:HG2	1.69	0.72
3:A:18:PRO:HG2	3:A:21:VAL:HG21	1.71	0.72
3:B:18:PRO:HG2	3:B:21:VAL:HG21	1.74	0.70
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.75	0.68
2:I:66:ARG:HB2	2:I:83:SER:HB2	1.76	0.68
2:H:68:THR:HG23	2:H:81:LYS:HB3	1.76	0.67
2:I:38:ARG:HB3	2:I:48:ILE:HD11	1.77	0.66
3:B:10:SER:HB2	3:B:108:PHE:H	1.60	0.65
2:H:86:THR:HG22	2:H:88:ALA:H	1.66	0.60
2:I:72:ASP:HB3	2:I:77:GLN:HG3	1.83	0.59
2:H:6:GLU:HG3	2:H:22:CYS:HB2	1.87	0.57
2:I:6:GLU:HG3	2:I:22:CYS:HB2	1.88	0.55
1:M:39:GLN:HB2	1:M:49:LEU:HD11	1.89	0.54
1:L:39:GLN:HB2	1:L:49:LEU:HD11	1.89	0.54
2:I:19:ARG:HH21	2:H:19:ARG:HH11	1.56	0.53
3:A:143:CYS:HB3	3:A:156:CYS:SG	2.50	0.51
2:I:65:GLU:H	2:I:65:GLU:CD	2.19	0.50
1:M:41:LYS:HD3	1:M:86:ALA:HB2	1.94	0.49
1:L:38:TYR:HE1	1:L:91:HIS:HB3	1.77	0.49
2:I:68:THR:HG23	2:I:81:LYS:HB3	1.94	0.48
2:H:18:LEU:HD22	2:H:82:LEU:HB3	1.95	0.48
1:L:68:GLY:HA3	1:L:73:PHE:HA	1.96	0.47
1:M:38:TYR:HE1	1:M:91:HIS:HB3	1.80	0.46
1:M:52:SER:HB2	1:M:55:ILE:HD12	1.98	0.46
2:I:6:GLU:OE1	2:I:111:GLY:HA3	2.16	0.46
2:I:85:VAL:HG13	2:I:89:ASP:HB2	1.98	0.46
3:B:96:LYS:HB3	3:B:96:LYS:HE3	1.70	0.46
3:B:136:ILE:HG21	3:A:136:ILE:HG21	1.98	0.46
1:L:40:GLN:O	1:L:86:ALA:HB1	2.16	0.45
2:I:63:ALA:O	2:I:67:VAL:HB	2.17	0.45
1:L:52:SER:HB2	1:L:55:ILE:HD12	1.99	0.44
2:H:6:GLU:OE2	2:H:111:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:ILE:HD12	1:L:75:LEU:HD23	1.99	0.44
1:M:21:ILE:HD12	1:M:75:LEU:HD23	1.98	0.44
3:A:43:ASP:OD1	3:A:70:GLN:HG2	2.17	0.44
3:A:11:PRO:HB2	3:A:18:PRO:HD2	1.99	0.44
2:I:90:THR:HA	2:I:116:VAL:O	2.18	0.44
1:M:40:GLN:O	1:M:86:ALA:HB1	2.18	0.44
2:I:93:TYR:O	2:I:113:GLY:HA2	2.18	0.44
2:H:62:TRP:CE3	2:H:63:ALA:HB2	2.53	0.44
2:H:48:ILE:HG12	2:H:62:TRP:HH2	1.84	0.42
3:B:50:CYS:HB2	3:B:66:ARG:HD3	2.00	0.42
1:M:18:ARG:HA	1:M:77:ILE:O	2.20	0.42
3:A:154:LYS:HE2	3:A:154:LYS:HB2	1.93	0.42
2:I:67:VAL:HG22	2:I:82:LEU:HD13	2.01	0.42
3:B:129:SER:OG	3:B:155:ASN:HA	2.19	0.41
3:B:103:GLU:HB2	3:B:105:PHE:CE2	2.54	0.41
2:H:59:TYR:CE1	2:H:67:VAL:HG12	2.55	0.41
2:H:93:TYR:O	2:H:113:GLY:HA2	2.20	0.41
3:B:8:ILE:HD11	3:B:27:ILE:HD11	2.03	0.41
2:H:18:LEU:HD12	2:H:116:VAL:HG11	2.03	0.41
2:H:24:ALA:HB2	2:H:29:PHE:CE1	2.56	0.41
3:A:96:LYS:HB2	3:A:96:LYS:HE3	1.86	0.41
2:H:81:LYS:HA	2:H:81:LYS:HD2	1.95	0.41
2:H:18:LEU:HB2	2:H:85:VAL:HG21	2.02	0.41
3:A:29:VAL:HG22	3:A:89:ASN:HA	2.02	0.41
2:H:67:VAL:CG2	2:H:82:LEU:HD13	2.51	0.40
3:A:149:LEU:HD12	3:A:149:LEU:HA	1.94	0.40
2:I:90:THR:HG23	2:I:117:THR:HA	2.03	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	L	108/220 (49%)	103 (95%)	5 (5%)	0	100	100
1	M	108/220 (49%)	104 (96%)	4 (4%)	0	100	100
2	H	109/225 (48%)	104 (95%)	5 (5%)	0	100	100
2	I	109/225 (48%)	103 (94%)	6 (6%)	0	100	100
3	A	150/290 (52%)	143 (95%)	7 (5%)	0	100	100
3	B	150/290 (52%)	145 (97%)	5 (3%)	0	100	100
All	All	734/1470 (50%)	702 (96%)	32 (4%)	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	L	94/193 (49%)	91 (97%)	3 (3%)	34	60
1	M	94/193 (49%)	90 (96%)	4 (4%)	25	49
2	H	90/190 (47%)	89 (99%)	1 (1%)	70	86
2	I	90/190 (47%)	89 (99%)	1 (1%)	70	86
3	A	139/252 (55%)	137 (99%)	2 (1%)	62	82
3	B	139/252 (55%)	135 (97%)	4 (3%)	37	64
All	All	646/1270 (51%)	631 (98%)	15 (2%)	46	71

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	18	ARG
1	L	22	THR
1	L	112	ILE
1	M	5	THR
1	M	18	ARG
1	M	22	THR
1	M	112	ILE

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Mol	Chain	Res	Type
2	I	19	ARG
3	B	21	VAL
3	B	61	ASP
3	B	70	GLN
3	B	96	LYS
2	H	90	THR
3	A	21	VAL
3	A	92	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	39	GLN
1	L	81	GLN
1	M	39	GLN
3	B	15	GLN
3	B	56	GLN
3	B	118	ASN
3	B	130	HIS
2	H	13	GLN
2	H	108	HIS
3	A	70	GLN
3	A	133	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

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.