



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:18 AM UTC

PDB ID : 1T60 / pdb_00001t60
Title : Crystal structure of Type IV collagen NC1 domain from bovine lens capsule
Authors : Vanacore, R.M.; Shanmugasundararaj, S.; Friedman, D.B.; Bondar, O.; Hudson, B.G.; Sundaramoorthy, M.
Deposited on : 2004-05-05
Resolution : 1.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

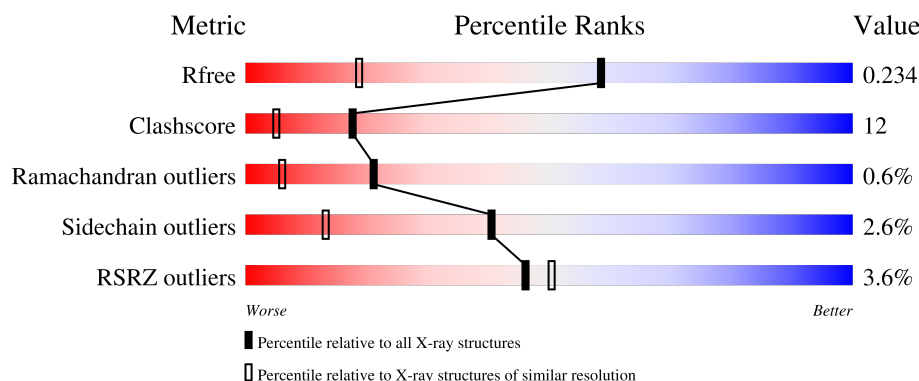
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	229	 76% 21% ..
1	B	229	 4% 73% 24% ..
1	D	229	 3% 74% 22% ..
1	E	229	 2% 76% 21% ..
1	G	229	 4% 79% 18% .

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Mol	Chain	Length	Quality of chain
1	H	229	
1	J	229	
1	K	229	
1	M	229	
1	N	229	
1	P	229	
1	Q	229	
1	S	229	
1	T	229	
1	V	229	
1	W	229	
2	C	227	
2	F	227	
2	I	227	
2	L	227	
2	O	227	
2	R	227	
2	U	227	
2	X	227	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	P	5006	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 44599 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 type iv collagen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1724	1085	300	318	21			
1	B	225	Total	C	N	O	S	0	0	0
			1745	1097	307	320	21			
1	D	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			
1	E	224	Total	C	N	O	S	0	0	0
			1735	1091	304	319	21			
1	G	228	Total	C	N	O	S	0	0	0
			1767	1110	310	326	21			
1	H	227	Total	C	N	O	S	0	0	0
			1760	1105	309	325	21			
1	J	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			
1	K	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			
1	M	223	Total	C	N	O	S	0	0	0
			1724	1085	300	318	21			
1	N	224	Total	C	N	O	S	0	0	0
			1738	1093	304	320	21			
1	P	225	Total	C	N	O	S	0	0	0
			1745	1097	307	320	21			
1	Q	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			
1	S	225	Total	C	N	O	S	0	0	0
			1745	1097	307	320	21			
1	T	227	Total	C	N	O	S	0	0	0
			1760	1105	309	325	21			
1	V	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			
1	W	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			

- Molecule 2 is a protein called type iv collagen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	223	Total	C	N	O	S	0	0	0
			1724	1093	291	321	19			
2	F	222	Total	C	N	O	S	0	0	0
			1720	1089	291	321	19			
2	I	225	Total	C	N	O	S	0	0	0
			1738	1100	294	325	19			
2	L	221	Total	C	N	O	S	0	0	0
			1708	1080	290	319	19			
2	O	224	Total	C	N	O	S	0	0	0
			1732	1097	293	323	19			
2	R	224	Total	C	N	O	S	0	0	0
			1732	1097	293	323	19			
2	U	224	Total	C	N	O	S	0	0	0
			1732	1097	293	323	19			
2	X	223	Total	C	N	O	S	0	0	0
			1724	1091	292	322	19			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

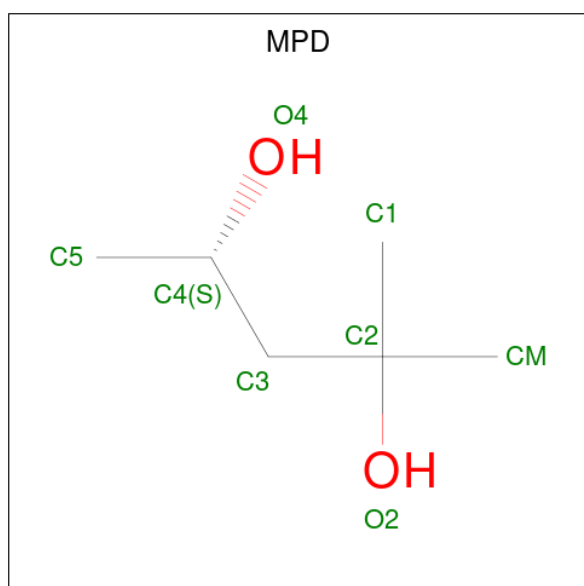
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	I	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		
3	L	1	Total	Cl	0	0
			1	1		
3	M	1	Total	Cl	0	0
			1	1		
3	O	1	Total	Cl	0	0
			1	1		
3	P	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	1	Total	Cl	0	0
			1	1		
3	S	1	Total	Cl	0	0
			1	1		
3	U	1	Total	Cl	0	0
			1	1		
3	V	1	Total	Cl	0	0
			1	1		
3	X	1	Total	Cl	0	0
			1	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	J	1	Total	C	O	0	0
			8	6	2		
4	M	1	Total	C	O	0	0
			8	6	2		
4	M	1	Total	C	O	0	0
			8	6	2		
4	P	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	C	O	0	0
			8	6	2		
4	S	1	Total	C	O	0	0
			8	6	2		
4	T	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	K	0	0
			1	1		
5	C	2	Total	K	0	0
			2	2		
5	D	1	Total	K	0	0
			1	1		
5	G	1	Total	K	0	0
			1	1		
5	H	1	Total	K	0	0
			1	1		
5	I	1	Total	K	0	0
			1	1		
5	L	1	Total	K	0	0
			1	1		
5	M	1	Total	K	0	0
			1	1		
5	N	1	Total	K	0	0
			1	1		
5	O	1	Total	K	0	0
			1	1		
5	P	1	Total	K	0	0
			1	1		
5	T	1	Total	K	0	0
			1	1		
5	U	2	Total	K	0	0
			2	2		
5	V	1	Total	K	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	112	Total O 112 112	0	0
6	B	101	Total O 101 101	0	0
6	C	116	Total O 116 116	0	0
6	D	134	Total O 134 134	0	0
6	E	127	Total O 127 127	0	0
6	F	117	Total O 117 117	0	0
6	G	144	Total O 144 144	0	0
6	H	104	Total O 104 104	0	0
6	I	121	Total O 121 121	0	0
6	J	97	Total O 97 97	0	0
6	K	102	Total O 102 102	0	0
6	L	111	Total O 111 111	0	0
6	M	118	Total O 118 118	0	0
6	N	113	Total O 113 113	0	0
6	O	125	Total O 125 125	0	0
6	P	133	Total O 133 133	0	0
6	Q	108	Total O 108 108	0	0
6	R	129	Total O 129 129	0	0
6	S	137	Total O 137 137	0	0
6	T	127	Total O 127 127	0	0
6	U	139	Total O 139 139	0	0
6	V	110	Total O 110 110	0	0

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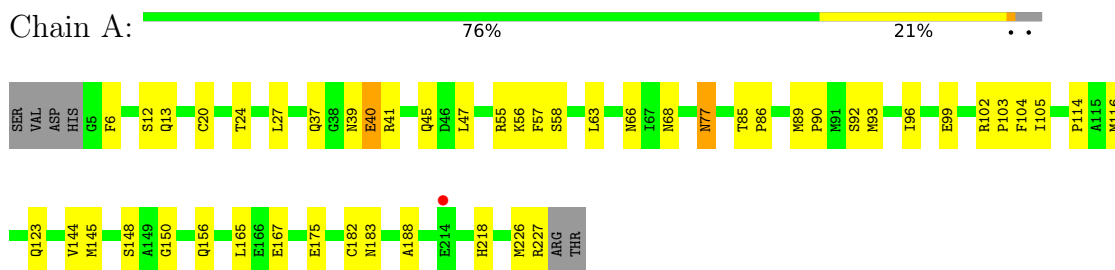
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	W	103	Total 103	O 103	0	0
6	X	110	Total 110	O 110	0	0

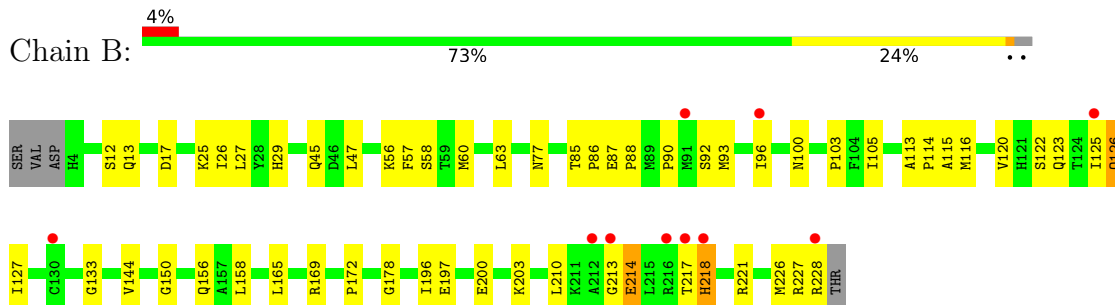
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

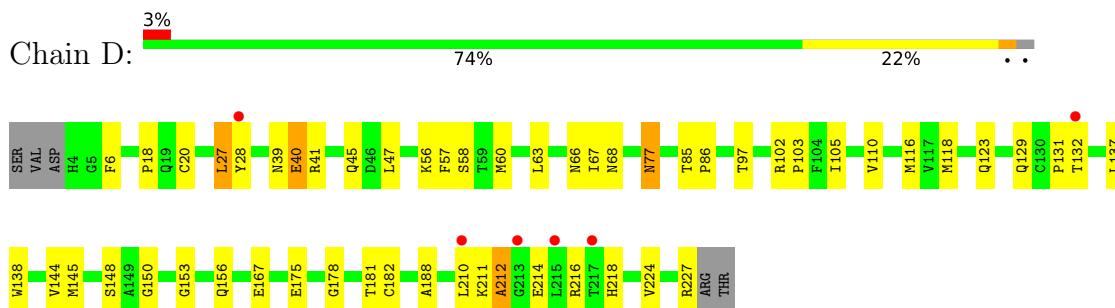
- Molecule 1: type iv collagen



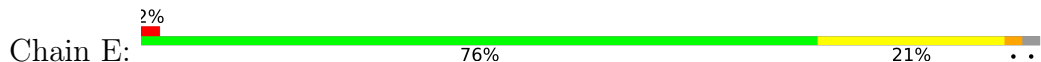
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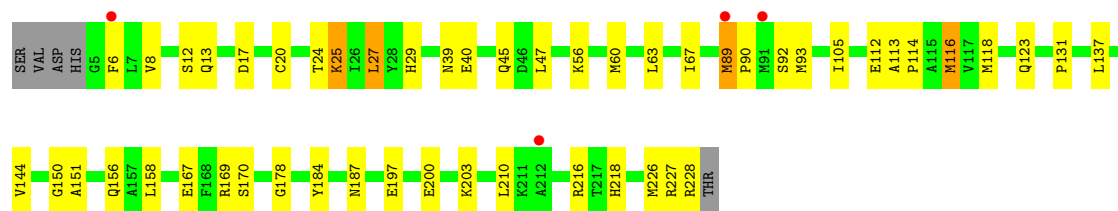


- Molecule 1: type iv collagen

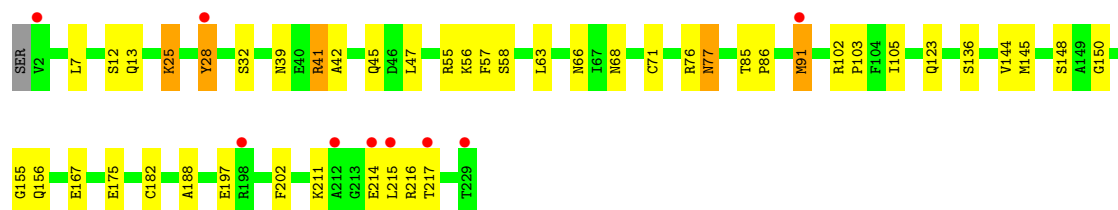
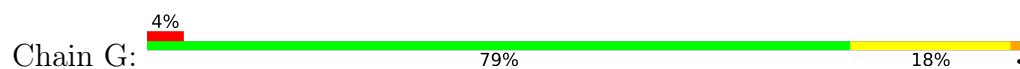


- Molecule 1: type iv collagen

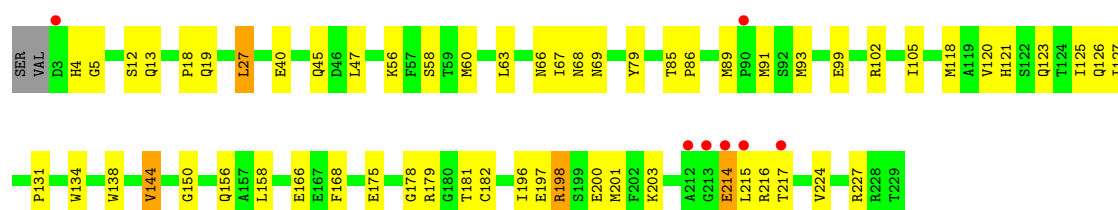
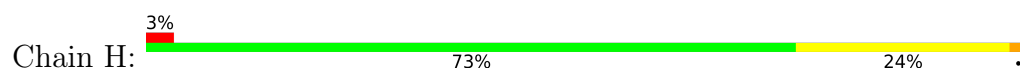




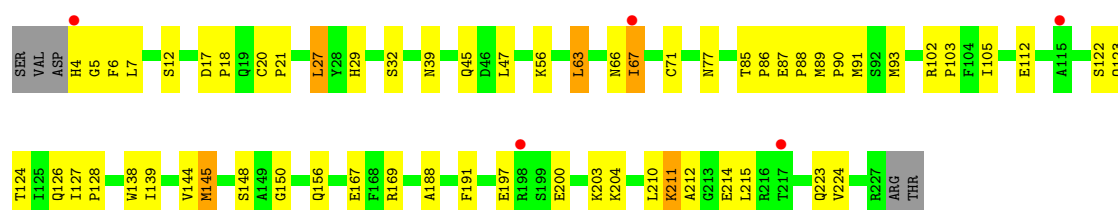
• Molecule 1: type iv collagen



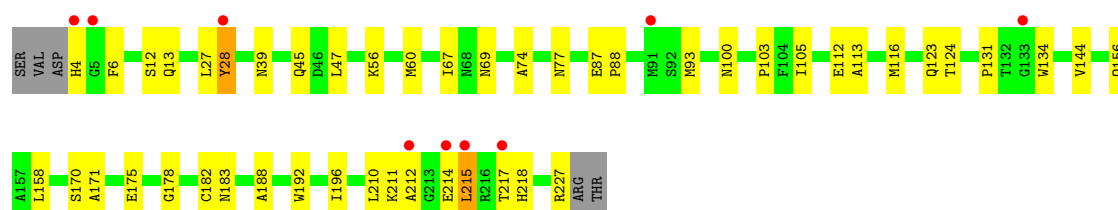
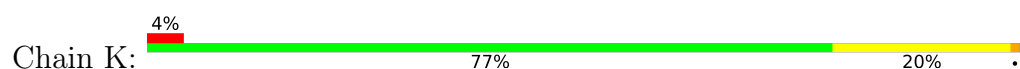
• Molecule 1: type iv collagen



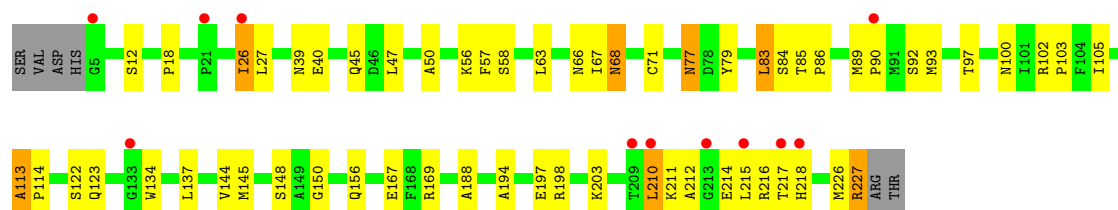
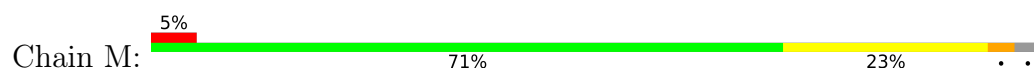
• Molecule 1: type iv collagen



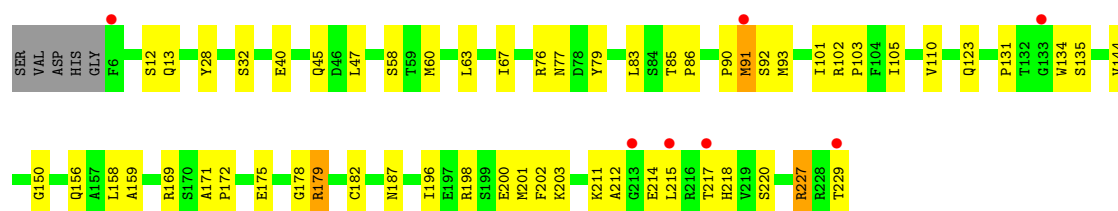
• Molecule 1: type iv collagen



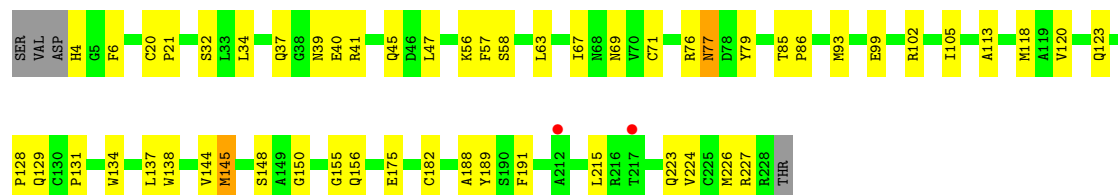
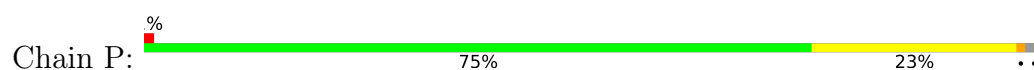
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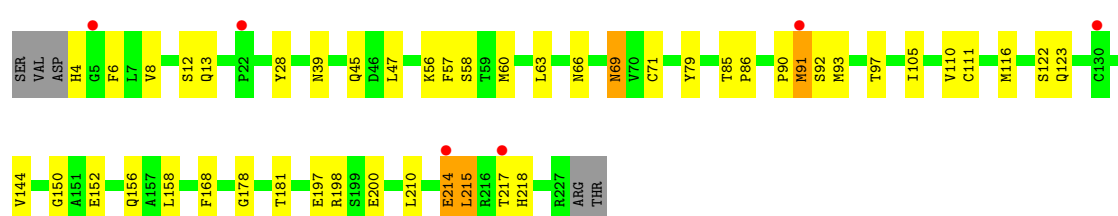
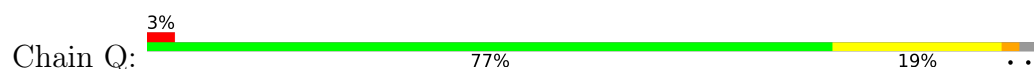
- Molecule 1: type iv collagen



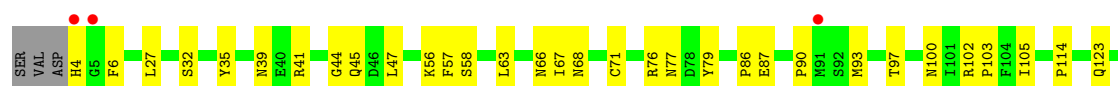
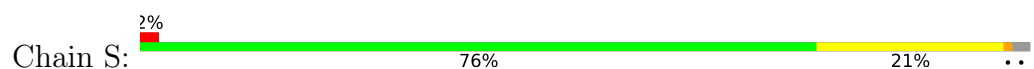
- Molecule 1: type iv collagen



- Molecule 1: type iv collagen

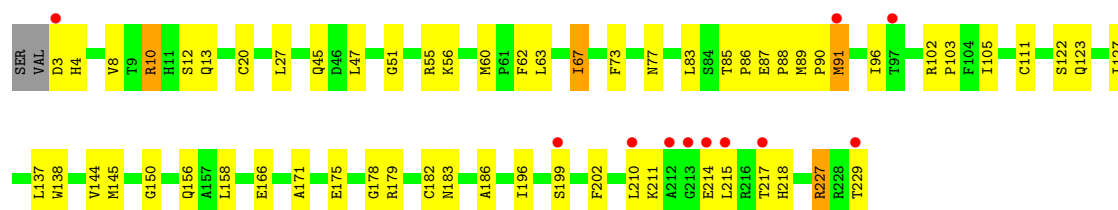


- Molecule 1: type iv collagen

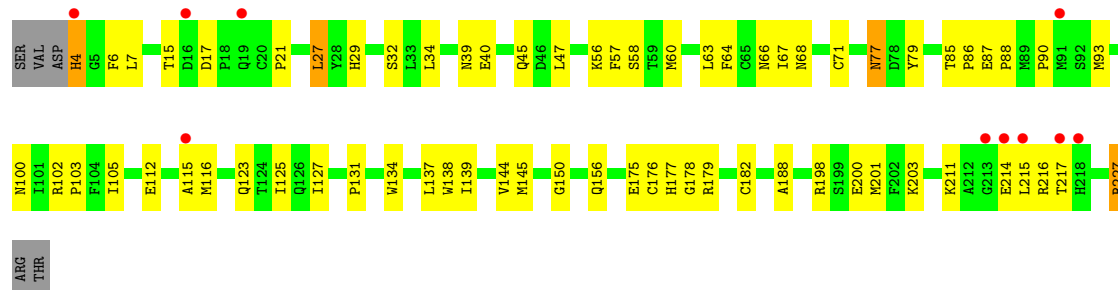




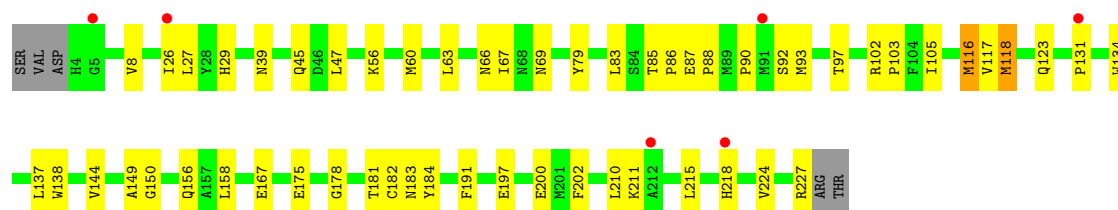
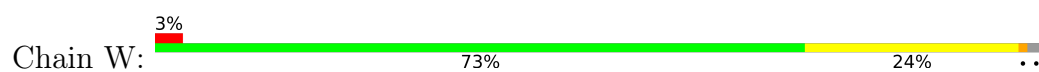
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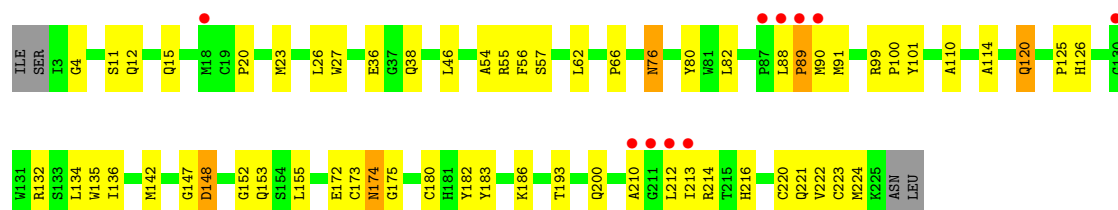
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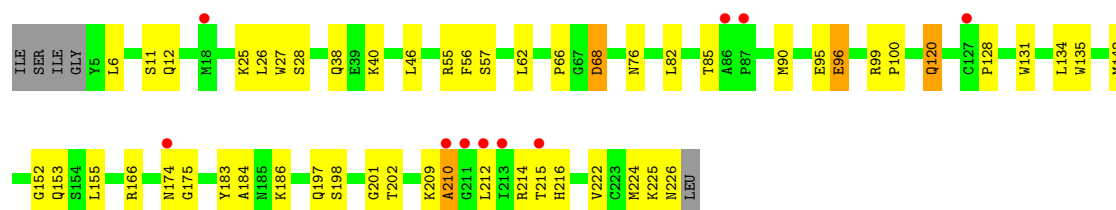
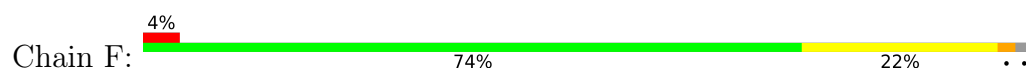
- Molecule 1: type iv collagen



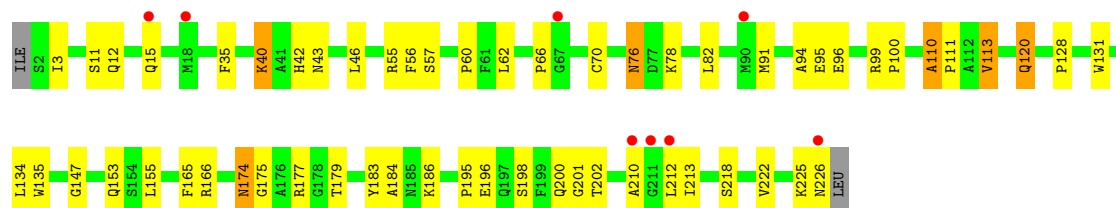
- Molecule 2: type iv collagen



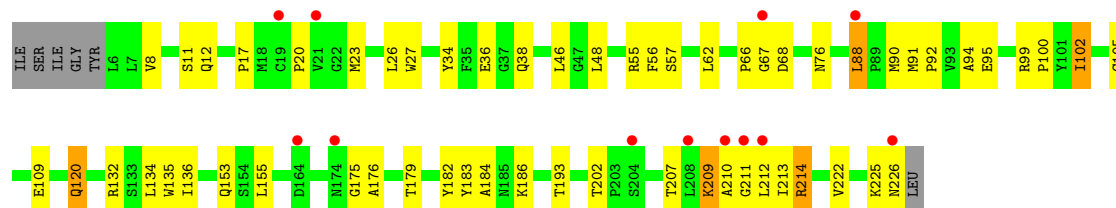
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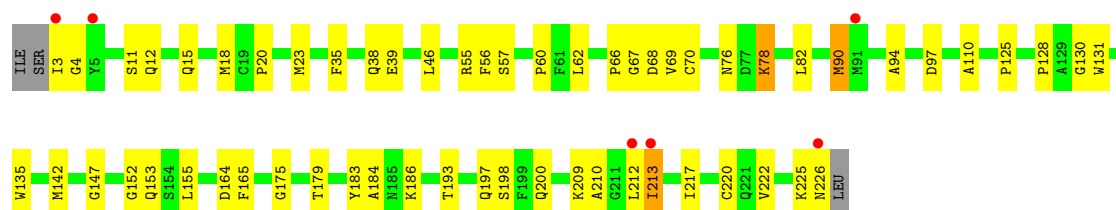
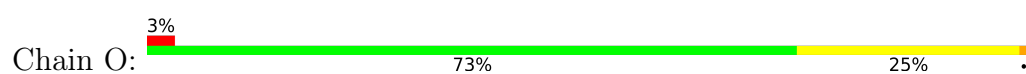
- Molecule 2: type iv collagen



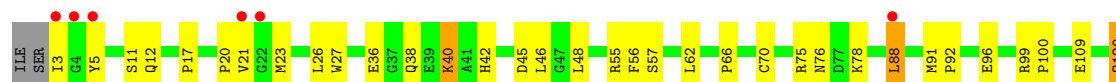
- Molecule 2: type iv collagen



- Molecule 2: type iv collagen

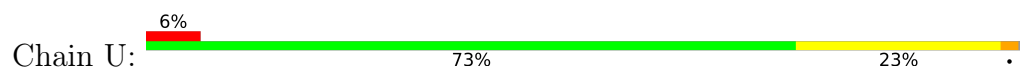


- Molecule 2: type iv collagen

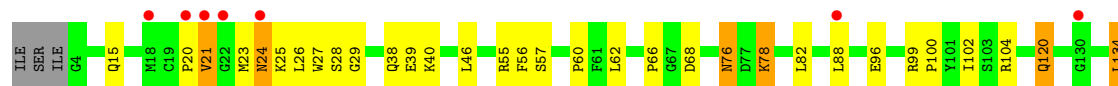
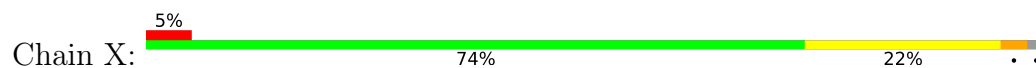




- Molecule 2: type iv collagen



- Molecule 2: type iv collagen



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.88Å 140.13Å 160.69Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	8.00 – 1.50 8.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-1.50) 89.1 (8.00-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.216 0.208 , 0.234	Depositor DCC
R_{free} test set	39655 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	44599	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9581e-04.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, CL, K

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	0.40	0/1774	0.91	3/2410 (0.1%)
1	B	0.38	0/1796	0.90	3/2439 (0.1%)
1	D	0.43	0/1785	0.93	7/2425 (0.3%)
1	E	0.40	0/1785	0.88	4/2424 (0.2%)
1	G	0.42	0/1818	0.90	4/2470 (0.2%)
1	H	0.39	0/1811	0.89	4/2460 (0.2%)
1	J	0.38	0/1785	0.92	4/2425 (0.2%)
1	K	0.38	0/1785	0.90	4/2425 (0.2%)
1	M	0.40	0/1774	0.92	7/2410 (0.3%)
1	N	0.38	0/1788	0.91	5/2429 (0.2%)
1	P	0.39	0/1796	0.90	4/2439 (0.2%)
1	Q	0.40	0/1785	0.90	2/2425 (0.1%)
1	S	0.40	0/1796	0.89	4/2439 (0.2%)
1	T	0.39	0/1811	0.88	6/2460 (0.2%)
1	V	0.37	0/1785	0.88	4/2425 (0.2%)
1	W	0.36	0/1785	0.88	3/2425 (0.1%)
2	C	0.41	0/1775	0.97	8/2415 (0.3%)
2	F	0.39	0/1771	0.89	2/2410 (0.1%)
2	I	0.39	0/1789	0.93	6/2434 (0.2%)
2	L	0.40	0/1758	0.93	5/2392 (0.2%)
2	O	0.39	0/1783	0.91	5/2426 (0.2%)
2	R	0.38	0/1783	0.92	3/2426 (0.1%)
2	U	0.39	0/1783	0.94	8/2426 (0.3%)
2	X	0.37	0/1775	0.93	5/2415 (0.2%)
All	All	0.39	0/42876	0.91	110/58274 (0.2%)

There are no bond length outliers.

The worst 5 of 110 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	217	THR	N-CA-C	-10.50	102.64	114.62
1	D	144	VAL	N-CA-C	8.86	119.08	111.90
1	S	144	VAL	N-CA-C	8.83	119.05	111.90
1	M	144	VAL	N-CA-C	8.47	118.76	111.90
1	P	144	VAL	N-CA-C	8.43	118.73	111.90

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	A	1724	0	1640	48	0
1	B	1745	0	1661	59	0
1	D	1734	0	1647	59	0
1	E	1735	0	1654	45	0
1	G	1767	0	1680	44	0
1	H	1760	0	1672	53	0
1	J	1734	0	1647	60	0
1	K	1734	0	1648	52	0
1	M	1724	0	1640	72	0
1	N	1738	0	1658	51	0
1	P	1745	0	1660	46	0
1	Q	1734	0	1648	43	0
1	S	1745	0	1661	51	0
1	T	1760	0	1672	57	0
1	V	1734	0	1647	59	0
1	W	1734	0	1648	51	0
2	C	1724	0	1637	57	0
2	F	1720	0	1629	44	0
2	I	1738	0	1648	57	0
2	L	1708	0	1619	43	0
2	O	1732	0	1643	47	0
2	R	1732	0	1643	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	U	1732	0	1643	52	0
2	X	1724	0	1631	55	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	X	1	0	0	0	0
4	A	8	0	14	0	0
4	D	8	0	14	1	0
4	J	8	0	14	3	0
4	M	16	0	28	1	0
4	P	8	0	14	7	0
4	S	16	0	28	5	0
4	T	8	0	14	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	T	1	0	0	0	0
5	U	2	0	0	0	0
5	V	1	0	0	0	0
6	A	112	0	0	3	0
6	B	101	0	0	1	0
6	C	116	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	134	0	0	3	0
6	E	127	0	0	1	0
6	F	117	0	0	0	0
6	G	144	0	0	1	0
6	H	104	0	0	2	0
6	I	121	0	0	2	0
6	J	97	0	0	1	0
6	K	102	0	0	1	0
6	L	111	0	0	0	0
6	M	118	0	0	2	0
6	N	113	0	0	5	0
6	O	125	0	0	2	0
6	P	133	0	0	3	0
6	Q	108	0	0	1	0
6	R	129	0	0	3	0
6	S	137	0	0	4	0
6	T	127	0	0	6	0
6	U	139	0	0	2	0
6	V	110	0	0	3	0
6	W	103	0	0	2	0
6	X	110	0	0	5	0
All	All	44599	0	39702	1007	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.

The worst 5 of 1007 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:203:LYS:HE2	1:B:203:LYS:HA	1.40	1.03
1:E:27:LEU:HD21	1:E:112:GLU:HG3	1.40	1.00
1:V:7:LEU:HD11	1:W:118:MET:HE2	1.52	0.90
1:V:123:GLN:HE22	2:X:55:ARG:H	1.20	0.89
1:N:200:GLU:HA	1:N:203:LYS:HE2	1.56	0.87

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 X-ray entries followed by that with respect to entries of similar resolution.

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	221/229 (96%)	214 (97%)	6 (3%)	1 (0%)	24	8
1	B	223/229 (97%)	213 (96%)	9 (4%)	1 (0%)	30	12
1	D	222/229 (97%)	211 (95%)	9 (4%)	2 (1%)	14	3
1	E	222/229 (97%)	213 (96%)	9 (4%)	0	100	100
1	G	226/229 (99%)	218 (96%)	6 (3%)	2 (1%)	14	3
1	H	225/229 (98%)	215 (96%)	9 (4%)	1 (0%)	30	12
1	J	222/229 (97%)	213 (96%)	8 (4%)	1 (0%)	24	8
1	K	222/229 (97%)	211 (95%)	10 (4%)	1 (0%)	24	8
1	M	221/229 (96%)	210 (95%)	10 (4%)	1 (0%)	24	8
1	N	222/229 (97%)	213 (96%)	7 (3%)	2 (1%)	14	3
1	P	223/229 (97%)	217 (97%)	4 (2%)	2 (1%)	14	3
1	Q	222/229 (97%)	212 (96%)	10 (4%)	0	100	100
1	S	223/229 (97%)	215 (96%)	7 (3%)	1 (0%)	30	12
1	T	225/229 (98%)	212 (94%)	13 (6%)	0	100	100
1	V	222/229 (97%)	209 (94%)	12 (5%)	1 (0%)	24	8
1	W	222/229 (97%)	210 (95%)	12 (5%)	0	100	100
2	C	221/227 (97%)	203 (92%)	17 (8%)	1 (0%)	24	8
2	F	220/227 (97%)	205 (93%)	13 (6%)	2 (1%)	14	3
2	I	223/227 (98%)	211 (95%)	10 (4%)	2 (1%)	14	3
2	L	219/227 (96%)	203 (93%)	15 (7%)	1 (0%)	24	8
2	O	222/227 (98%)	208 (94%)	11 (5%)	3 (1%)	9	1
2	R	222/227 (98%)	208 (94%)	12 (5%)	2 (1%)	14	3
2	U	222/227 (98%)	212 (96%)	9 (4%)	1 (0%)	24	8
2	X	221/227 (97%)	200 (90%)	19 (9%)	2 (1%)	14	3
All	All	5333/5480 (97%)	5056 (95%)	247 (5%)	30 (1%)	21	6

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	214	GLU
1	D	212	ALA
2	F	175	GLY
1	H	214	GLU
2	L	175	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	189/195 (97%)	185 (98%)	4 (2%)	47	19
1	B	191/195 (98%)	188 (98%)	3 (2%)	55	28
1	D	190/195 (97%)	186 (98%)	4 (2%)	47	19
1	E	190/195 (97%)	185 (97%)	5 (3%)	40	13
1	G	194/195 (100%)	188 (97%)	6 (3%)	35	9
1	H	193/195 (99%)	188 (97%)	5 (3%)	40	13
1	J	190/195 (97%)	185 (97%)	5 (3%)	40	13
1	K	190/195 (97%)	187 (98%)	3 (2%)	55	28
1	M	189/195 (97%)	181 (96%)	8 (4%)	26	4
1	N	191/195 (98%)	187 (98%)	4 (2%)	47	19
1	P	191/195 (98%)	188 (98%)	3 (2%)	55	28
1	Q	190/195 (97%)	186 (98%)	4 (2%)	47	19
1	S	191/195 (98%)	185 (97%)	6 (3%)	35	9
1	T	193/195 (99%)	188 (97%)	5 (3%)	40	13
1	V	190/195 (97%)	184 (97%)	6 (3%)	34	8
1	W	190/195 (97%)	186 (98%)	4 (2%)	47	19
2	C	187/191 (98%)	183 (98%)	4 (2%)	47	19
2	F	187/191 (98%)	182 (97%)	5 (3%)	39	12
2	I	189/191 (99%)	184 (97%)	5 (3%)	40	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	186/191 (97%)	178 (96%)	8 (4%)	26	4
2	O	188/191 (98%)	183 (97%)	5 (3%)	39	12
2	R	188/191 (98%)	183 (97%)	5 (3%)	39	12
2	U	188/191 (98%)	183 (97%)	5 (3%)	39	12
2	X	187/191 (98%)	181 (97%)	6 (3%)	34	8
All	All	4552/4648 (98%)	4434 (97%)	118 (3%)	40	13

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	26	ILE
1	W	116	MET
2	O	164	ASP
1	W	83	LEU
2	U	76	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 199 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	120	GLN
2	R	221	GLN
2	O	221	GLN
1	Q	29	HIS
1	S	123	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

Of 41 ligands modelled in this entry, 32 are monoatomic - leaving 9 for Mogul analysis.

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	MPD	S	5004	-	7,7,7	0.50	0	9,10,10	0.50	0
4	MPD	A	5001	-	7,7,7	0.49	0	9,10,10	0.51	0
4	MPD	T	5002	-	7,7,7	1.66	3 (42%)	9,10,10	1.14	0
4	MPD	S	5005	-	7,7,7	0.77	0	9,10,10	0.70	0
4	MPD	M	5008	-	7,7,7	0.62	0	9,10,10	0.46	0
4	MPD	P	5006	-	7,7,7	0.61	0	9,10,10	0.54	0
4	MPD	D	5007	-	7,7,7	0.89	0	9,10,10	0.52	0
4	MPD	J	5009	-	7,7,7	0.55	0	9,10,10	0.57	0
4	MPD	M	5003	-	7,7,7	0.57	0	9,10,10	0.55	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	MPD	S	5004	-	-	0/5/5/5	-
4	MPD	A	5001	-	-	0/5/5/5	-
4	MPD	T	5002	-	-	2/5/5/5	-
4	MPD	S	5005	-	-	0/5/5/5	-
4	MPD	M	5008	-	-	0/5/5/5	-
4	MPD	P	5006	-	-	0/5/5/5	-
4	MPD	D	5007	-	-	3/5/5/5	-
4	MPD	J	5009	-	-	0/5/5/5	-
4	MPD	M	5003	-	-	2/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	5002	MPD	CM-C2	-2.63	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	5002	MPD	C3-C2	-2.08	1.48	1.54
4	T	5002	MPD	C1-C2	-2.01	1.46	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	5007	MPD	C1-C2-C3-C4
4	D	5007	MPD	O2-C2-C3-C4
4	M	5003	MPD	C1-C2-C3-C4
4	D	5007	MPD	CM-C2-C3-C4
4	M	5003	MPD	CM-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	5005	MPD	5	0
4	M	5008	MPD	1	0
4	P	5006	MPD	7	0
4	D	5007	MPD	1	0
4	J	5009	MPD	3	0

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	223/229 (97%)	0.02	1 (0%) 88 90	10, 18, 33, 42	0
1	B	225/229 (98%)	0.21	10 (4%) 39 43	11, 19, 41, 49	0
1	D	224/229 (97%)	-0.19	6 (2%) 56 60	8, 14, 33, 49	0
1	E	224/229 (97%)	-0.12	4 (1%) 67 71	9, 16, 35, 45	0
1	G	228/229 (99%)	-0.13	9 (3%) 43 47	9, 15, 39, 47	0
1	H	227/229 (99%)	0.07	7 (3%) 51 55	10, 18, 39, 50	0
1	J	224/229 (97%)	0.15	5 (2%) 62 66	10, 20, 41, 49	0
1	K	224/229 (97%)	0.13	9 (4%) 42 46	10, 18, 41, 50	0
1	M	223/229 (97%)	0.18	11 (4%) 35 38	10, 20, 38, 50	0
1	N	224/229 (97%)	0.14	7 (3%) 51 55	10, 19, 41, 49	0
1	P	225/229 (98%)	-0.09	2 (0%) 81 84	10, 18, 32, 45	0
1	Q	224/229 (97%)	-0.01	6 (2%) 56 60	10, 18, 39, 47	0
1	S	225/229 (98%)	-0.08	4 (1%) 67 71	10, 17, 32, 42	0
1	T	227/229 (99%)	0.01	11 (4%) 35 39	10, 18, 42, 49	0
1	V	224/229 (97%)	0.39	10 (4%) 38 42	12, 22, 42, 50	0
1	W	224/229 (97%)	0.25	6 (2%) 56 60	10, 21, 43, 49	0
2	C	223/227 (98%)	0.27	10 (4%) 38 42	10, 20, 40, 50	0
2	F	222/227 (97%)	0.24	10 (4%) 38 42	9, 19, 38, 50	0
2	I	225/227 (99%)	0.22	8 (3%) 46 50	9, 20, 36, 48	0
2	L	221/227 (97%)	0.23	12 (5%) 31 34	11, 20, 41, 50	0
2	O	224/227 (98%)	-0.01	6 (2%) 56 60	9, 17, 34, 45	0
2	R	224/227 (98%)	0.07	15 (6%) 24 26	9, 17, 37, 50	0
2	U	224/227 (98%)	0.04	13 (5%) 29 31	9, 16, 37, 47	0
2	X	223/227 (98%)	0.33	11 (4%) 35 38	10, 20, 41, 50	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	5381/5480 (98%)	0.10	193 (3%)	46	50	8, 18, 39, 50	0

The worst 5 of 193 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	21	VAL	9.8
2	L	212	LEU	6.7
1	K	217	THR	5.8
2	I	210	ALA	5.6
1	D	28	TYR	5.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MPD	S	5005	8/8	0.40	0.19	47,49,49,50	0
4	MPD	P	5006	8/8	0.41	0.22	42,45,49,50	0
4	MPD	J	5009	8/8	0.55	0.20	46,48,50,50	0
4	MPD	M	5008	8/8	0.66	0.13	38,40,44,46	0
4	MPD	T	5002	8/8	0.66	0.14	45,46,47,47	0
4	MPD	D	5007	8/8	0.73	0.17	42,44,44,46	0
4	MPD	S	5004	8/8	0.75	0.12	45,45,46,47	0
4	MPD	A	5001	8/8	0.76	0.11	37,40,41,44	0
4	MPD	M	5003	8/8	0.91	0.07	24,29,31,33	0
5	K	M	5105	1/1	0.92	0.10	42,42,42,42	0
5	K	V	5108	1/1	0.95	0.07	36,36,36,36	0
5	K	P	5106	1/1	0.96	0.08	33,33,33,33	0
5	K	D	5102	1/1	0.96	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	K	H	5111	1/1	0.97	0.04	21,21,21,21	0
3	CL	V	5215	1/1	0.97	0.03	17,17,17,17	0
3	CL	S	5213	1/1	0.98	0.04	16,16,16,16	0
5	K	I	5112	1/1	0.98	0.04	21,21,21,21	0
5	K	L	5104	1/1	0.98	0.04	27,27,27,27	0
5	K	B	5109	1/1	0.98	0.03	20,20,20,20	0
5	K	C	5101	1/1	0.98	0.04	26,26,26,26	0
5	K	U	5116	1/1	0.98	0.03	18,18,18,18	0
3	CL	A	5201	1/1	0.98	0.03	13,13,13,13	0
3	CL	X	5216	1/1	0.99	0.02	18,18,18,18	0
3	CL	G	5205	1/1	0.99	0.03	14,14,14,14	0
5	K	C	5110	1/1	0.99	0.03	19,19,19,19	0
3	CL	J	5207	1/1	0.99	0.03	13,13,13,13	0
5	K	G	5103	1/1	0.99	0.05	34,34,34,34	0
3	CL	L	5209	1/1	0.99	0.02	15,15,15,15	0
3	CL	M	5208	1/1	0.99	0.05	15,15,15,15	0
3	CL	O	5210	1/1	0.99	0.02	13,13,13,13	0
3	CL	P	5211	1/1	0.99	0.03	13,13,13,13	0
3	CL	R	5212	1/1	0.99	0.03	14,14,14,14	0
5	K	T	5115	1/1	0.99	0.03	17,17,17,17	0
5	K	U	5107	1/1	0.99	0.06	30,30,30,30	0
3	CL	C	5202	1/1	0.99	0.02	15,15,15,15	0
3	CL	F	5204	1/1	0.99	0.01	14,14,14,14	0
3	CL	U	5214	1/1	1.00	0.02	12,12,12,12	0
3	CL	I	5206	1/1	1.00	0.03	11,11,11,11	0
3	CL	D	5203	1/1	1.00	0.03	13,13,13,13	0
5	K	N	5113	1/1	1.00	0.03	15,15,15,15	0
5	K	O	5114	1/1	1.00	0.02	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.