



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 04:47 PM EDT

PDB ID : 5NB0  
Title : Crystal structures of homooligomers of collagen type IV. alpha3NC1  
Authors : Casino, P.; Marina, A.  
Deposited on : 2017-02-28  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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

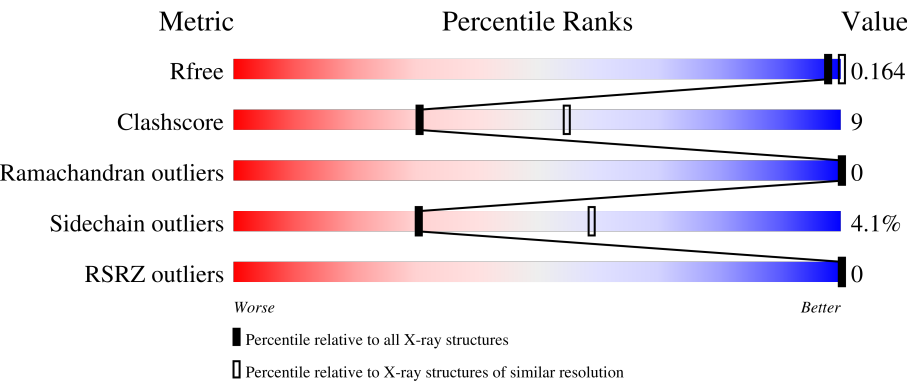
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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 <sub>free</sub>	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	230	<div><div>86%</div><div>10%</div><div>..</div></div>
1	B	230	<div><div>83%</div><div>14%</div><div>..</div></div>
1	C	230	<div><div>80%</div><div>15%</div><div>..</div></div>
1	D	230	<div><div>80%</div><div>17%</div><div>..</div></div>
1	E	230	<div><div>82%</div><div>15%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	230	 82% 15% . .
1	G	230	 80% 17% . .
1	H	230	 80% 15% . .

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
2	CL	A	301	-	-	X	-
2	CL	C	301	-	-	X	-
2	CL	D	301	-	-	X	-
2	CL	F	301	-	-	X	-
2	CL	G	301	-	-	X	-
2	CL	H	301	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14139 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 Collagen alpha-3(IV) chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1735	1105	295	316	19			
1	B	226	Total	C	N	O	S	0	1	0
			1743	1110	295	318	20			
1	C	225	Total	C	N	O	S	0	0	0
			1731	1102	294	316	19			
1	D	227	Total	C	N	O	S	0	0	0
			1749	1112	299	319	19			
1	E	225	Total	C	N	O	S	0	0	0
			1731	1102	294	316	19			
1	F	226	Total	C	N	O	S	0	0	0
			1740	1106	297	318	19			
1	G	225	Total	C	N	O	S	0	0	0
			1731	1102	294	316	19			
1	H	225	Total	C	N	O	S	0	0	0
			1731	1102	294	316	19			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cl	0	0
			3	3		
2	B	3	Total	Cl	0	0
			3	3		
2	C	2	Total	Cl	0	0
			2	2		
2	D	1	Total	Cl	0	0
			1	1		
2	E	1	Total	Cl	0	0
			1	1		
2	F	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total 3	Cl 3	0	0
2	H	1	Total 1	Cl 1	0	0


- Molecule 3 is water.

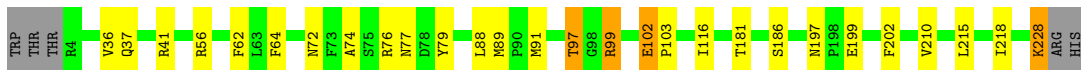
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total 32	O 32	0	0
3	B	33	Total 33	O 33	0	0
3	C	25	Total 25	O 25	0	0
3	D	31	Total 31	O 31	0	0
3	E	31	Total 31	O 31	0	0
3	F	29	Total 29	O 29	0	0
3	G	23	Total 23	O 23	0	0
3	H	28	Total 28	O 28	0	0

### 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.

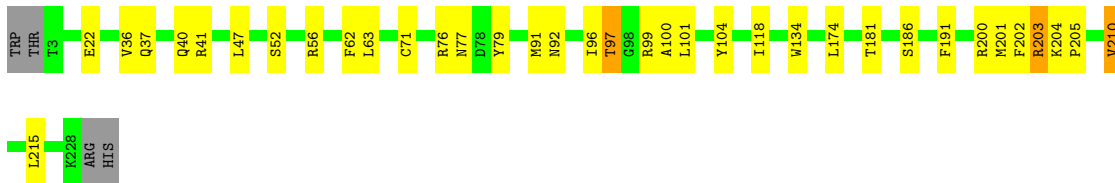
- Molecule 1: Collagen alpha-3(IV) chain

Chain A: 




- Molecule 1: Collagen alpha-3(IV) chain

Chain B: 




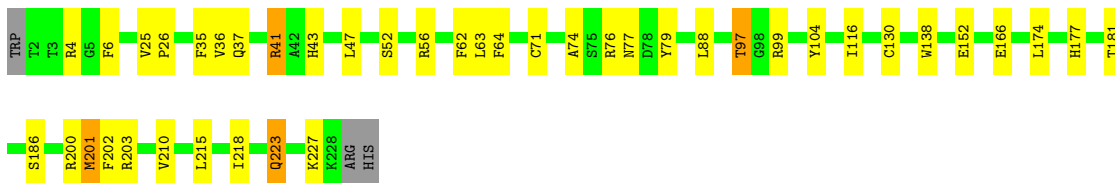
- Molecule 1: Collagen alpha-3(IV) chain

Chain C: 




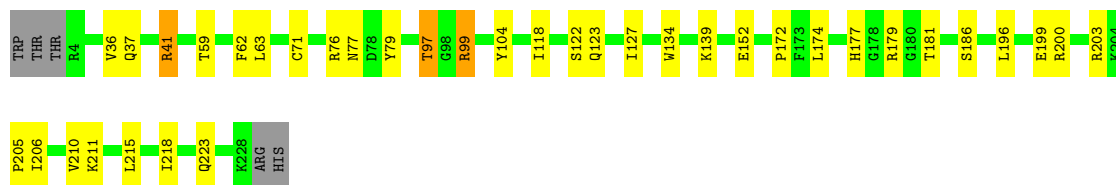
- Molecule 1: Collagen alpha-3(IV) chain

Chain D: 




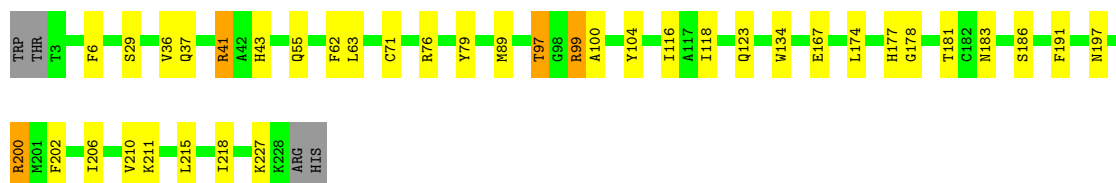
- Molecule 1: Collagen alpha-3(IV) chain

Chain E:  82% 15% ..




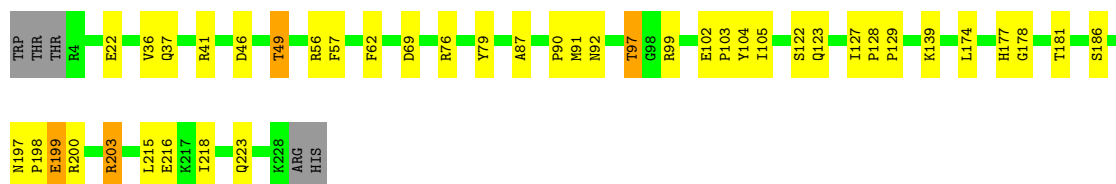
- Molecule 1: Collagen alpha-3(IV) chain

Chain F:  82% 15% ..




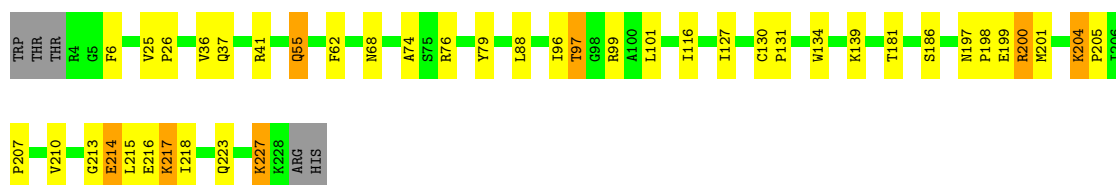
- Molecule 1: Collagen alpha-3(IV) chain

Chain G:  80% 17% ..



- Molecule 1: Collagen alpha-3(IV) chain

Chain H:  80% 15% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.52Å 131.52Å 248.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.78 – 2.70 51.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (51.78-2.70) 98.3 (51.78-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.12 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.163 , 0.176 0.164 , 0.164	Depositor DCC
$R_{free}$ test set	2206 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 7.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.468 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.503 for H, K, L 0.497 for K, H, -L	Depositor
Outliers	0 of 43349 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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 24.44 % 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 3.8360e-03.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

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

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

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	0.41	0/1787	0.55	0/2428
1	B	0.43	0/1798	0.60	0/2444
1	C	0.46	0/1783	0.60	0/2424
1	D	0.45	0/1801	0.58	0/2448
1	E	0.40	0/1783	0.55	0/2424
1	F	0.42	0/1792	0.58	0/2437
1	G	0.40	0/1783	0.56	0/2424
1	H	0.44	0/1783	0.58	0/2424
All	All	0.43	0/14310	0.58	0/19453

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	1735	0	1662	24	0
1	B	1743	0	1667	44	0
1	C	1731	0	1651	58	0
1	D	1749	0	1671	32	0
1	E	1731	0	1651	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1740	0	1658	38	1
1	G	1731	0	1651	28	1
1	H	1731	0	1651	54	0
2	A	3	0	0	2	0
2	B	3	0	0	1	0
2	C	2	0	0	2	0
2	D	1	0	0	2	0
2	E	1	0	0	1	0
2	F	2	0	0	2	0
2	G	3	0	0	2	0
2	H	1	0	0	2	0
3	A	32	0	0	1	0
3	B	33	0	0	3	0
3	C	25	0	0	0	0
3	D	31	0	0	2	0
3	E	31	0	0	4	0
3	F	29	0	0	3	0
3	G	23	0	0	2	0
3	H	28	0	0	2	0
All	All	14139	0	13262	250	1

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 9.

All (250) 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:C:89:MET:HE2	1:C:104:TYR:CE2	1.40	1.54
1:C:199:GLU:HG2	1:H:216:GLU:CG	1.37	1.49
1:C:89:MET:CE	1:C:104:TYR:CE2	1.97	1.48
1:C:199:GLU:CG	1:H:216:GLU:HG3	1.57	1.33
1:C:91:MET:O	1:E:211:LYS:NZ	1.68	1.26
1:D:41:ARG:NH1	1:D:152:GLU:OE1	1.66	1.24
1:B:99:ARG:HB2	1:H:88:LEU:HD11	1.23	1.15
1:B:99:ARG:CB	1:H:88:LEU:HD11	1.78	1.12
1:C:199:GLU:CG	1:H:216:GLU:CG	2.25	1.05
1:C:89:MET:HE1	1:C:104:TYR:CE2	1.91	1.02
1:B:203:ARG:HH11	1:B:203:ARG:CG	1.75	0.99
1:A:197:ASN:OD1	1:A:199:GLU:HG2	1.63	0.97
1:C:197:ASN:HB2	1:H:213:GLY:O	1.64	0.97
1:H:96:ILE:HD11	1:H:101:LEU:HD23	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLU:CB	1:H:216:GLU:HG3	1.97	0.94
1:C:89:MET:CE	1:C:104:TYR:CD2	2.52	0.92
1:C:199:GLU:HG2	1:H:216:GLU:CB	2.00	0.91
1:A:76:ARG:O	2:A:301:CL:CL	2.25	0.91
1:C:136:SER:OG	1:C:223:GLN:NE2	2.03	0.91
1:B:99:ARG:HB2	1:H:88:LEU:CD1	2.02	0.90
1:C:199:GLU:HG2	1:H:216:GLU:HG3	0.90	0.90
1:D:76:ARG:O	2:D:301:CL:CL	2.27	0.89
1:B:203:ARG:HH11	1:B:203:ARG:HG2	1.39	0.88
1:B:99:ARG:CB	1:H:88:LEU:CD1	2.54	0.84
1:C:199:GLU:HG2	1:H:216:GLU:CD	1.99	0.82
1:H:76:ARG:O	2:H:301:CL:CL	2.34	0.82
1:F:99:ARG:HD2	1:F:99:ARG:C	1.99	0.82
1:B:56:ARG:NH2	1:C:198:PRO:O	2.14	0.80
1:C:89:MET:HE1	1:C:104:TYR:CZ	2.16	0.80
1:B:76:ARG:O	2:B:301:CL:CL	2.37	0.79
1:C:199:GLU:CG	1:H:216:GLU:CD	2.51	0.77
1:C:89:MET:CE	1:C:104:TYR:CZ	2.65	0.77
1:B:92:ASN:OD1	3:B:401:HOH:O	2.01	0.77
1:E:139:LYS:HE2	1:E:223:GLN:OE1	1.87	0.75
1:H:37:GLN:HB2	1:H:79:TYR:HB2	1.68	0.74
1:F:37:GLN:HB2	1:F:79:TYR:HB2	1.71	0.73
1:C:89:MET:HE2	1:C:104:TYR:HE2	0.93	0.72
1:G:127:ILE:CG2	1:G:223:GLN:HE21	2.02	0.72
1:D:37:GLN:HB2	1:D:79:TYR:HB2	1.70	0.71
1:E:37:GLN:HB2	1:E:79:TYR:HB2	1.72	0.71
1:B:99:ARG:HB3	1:H:88:LEU:CD1	2.21	0.70
1:B:99:ARG:HB3	1:H:88:LEU:HD11	1.71	0.70
1:A:37:GLN:HB2	1:A:79:TYR:HB2	1.73	0.70
1:G:76:ARG:O	2:G:301:CL:CL	2.47	0.70
1:B:97:THR:HG22	1:B:181:THR:HG22	1.74	0.70
1:E:99:ARG:HD3	1:G:87:ALA:HA	1.74	0.69
1:F:76:ARG:O	2:F:301:CL:CL	2.48	0.69
1:B:203:ARG:HH11	1:B:203:ARG:HG3	1.57	0.69
1:E:127:ILE:HG21	1:E:139:LYS:HD3	1.75	0.69
1:C:37:GLN:HB2	1:C:79:TYR:HB2	1.74	0.68
1:E:127:ILE:HG21	1:E:139:LYS:CD	2.24	0.68
1:G:215:LEU:O	1:G:218:ILE:HG13	1.93	0.68
1:B:37:GLN:HB2	1:B:79:TYR:HB2	1.75	0.68
1:B:200:ARG:NH2	1:B:203:ARG:HB3	2.09	0.68
1:G:37:GLN:HB2	1:G:79:TYR:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:GLN:HE22	1:E:37:GLN:HE22	1.39	0.68
1:B:99:ARG:NH2	1:C:201:MET:O	2.27	0.67
1:H:217:LYS:HG3	1:H:218:ILE:HG23	1.75	0.67
1:B:204:LYS:HG2	1:B:205:PRO:O	1.94	0.66
1:G:127:ILE:HG21	1:G:223:GLN:HE21	1.60	0.66
1:B:203:ARG:CG	1:B:203:ARG:NH1	2.45	0.66
1:H:96:ILE:CD1	1:H:101:LEU:HD23	2.24	0.66
1:C:97:THR:HG22	1:C:181:THR:HG22	1.79	0.65
1:G:97:THR:HG22	1:G:181:THR:HG22	1.79	0.65
1:G:46:ASP:HB3	1:G:49:THR:HG23	1.77	0.64
1:H:214:GLU:O	1:H:217:LYS:HG2	1.98	0.64
1:F:178:GLY:HA3	2:F:301:CL:CL	2.34	0.64
1:F:97:THR:HG22	1:F:181:THR:HG22	1.81	0.64
1:C:199:GLU:HB3	1:H:216:GLU:OE1	1.98	0.63
1:B:203:ARG:HG3	1:B:203:ARG:NH1	2.12	0.63
1:A:202:PHE:HB3	1:C:99:ARG:HA	1.80	0.63
1:H:217:LYS:NZ	3:H:401:HOH:O	2.27	0.63
1:E:127:ILE:HG21	1:E:139:LYS:CE	2.29	0.63
1:E:122:SER:O	1:E:123:GLN:HB2	1.99	0.62
1:B:22:GLU:OE2	3:B:402:HOH:O	2.15	0.62
1:B:63:LEU:HD22	1:C:218:ILE:HD12	1.80	0.62
1:H:210:VAL:HG23	1:H:215:LEU:HD23	1.81	0.62
1:A:97:THR:HG22	1:A:181:THR:HG22	1.81	0.61
1:H:68:ASN:ND2	3:H:402:HOH:O	2.33	0.61
1:G:92:ASN:OD1	3:G:401:HOH:O	2.16	0.61
1:E:139:LYS:HG2	1:E:223:GLN:HG2	1.82	0.61
1:B:99:ARG:C	1:B:101:LEU:H	2.05	0.60
1:D:97:THR:HG22	1:D:181:THR:HG22	1.82	0.60
1:F:197:ASN:HB2	1:F:200:ARG:HG3	1.83	0.60
1:H:97:THR:HG22	1:H:181:THR:HG22	1.82	0.60
1:G:200:ARG:HG3	1:G:203:ARG:HG3	1.83	0.60
1:C:203:ARG:CG	1:C:203:ARG:HH11	2.14	0.60
1:B:77:ASN:O	1:E:77:ASN:ND2	2.33	0.60
1:C:198:PRO:HD2	1:C:199:GLU:OE1	2.02	0.60
1:G:215:LEU:O	1:G:218:ILE:CG1	2.50	0.59
1:C:199:GLU:CD	1:C:199:GLU:H	2.05	0.59
1:A:102:GLU:HG2	1:A:103:PRO:N	2.17	0.59
1:C:210:VAL:HG23	1:C:215:LEU:HD23	1.85	0.59
1:E:76:ARG:O	2:E:301:CL:CL	2.58	0.59
1:E:139:LYS:HG2	1:E:223:GLN:CG	2.32	0.58
1:F:197:ASN:HB2	1:F:200:ARG:CD	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:HE	1:B:203:ARG:NH1	2.01	0.58
1:C:76:ARG:O	2:C:301:CL:CL	2.58	0.58
1:C:197:ASN:CB	1:H:213:GLY:O	2.46	0.57
1:F:227:LYS:O	3:F:401:HOH:O	2.17	0.57
1:A:202:PHE:HB2	1:C:99:ARG:HG3	1.86	0.57
1:F:197:ASN:HB2	1:F:200:ARG:CG	2.36	0.56
1:A:88:LEU:HG	1:A:89:MET:N	2.21	0.56
1:E:205:PRO:HA	3:E:420:HOH:O	2.06	0.56
1:E:97:THR:HG22	1:E:181:THR:HG22	1.86	0.56
1:A:99:ARG:HH21	1:B:203:ARG:CZ	2.18	0.56
1:C:203:ARG:HH11	1:C:203:ARG:HG2	1.71	0.56
1:E:127:ILE:HG21	1:E:139:LYS:HE2	1.87	0.56
1:H:127:ILE:HD12	1:H:139:LYS:HD2	1.87	0.55
1:F:210:VAL:HG23	1:F:215:LEU:HD23	1.88	0.55
1:D:41:ARG:NH1	1:D:152:GLU:CD	2.55	0.55
1:E:139:LYS:CE	1:E:223:GLN:OE1	2.55	0.55
1:D:210:VAL:HG23	1:D:215:LEU:HD23	1.89	0.54
1:D:63:LEU:HD22	1:F:218:ILE:HD12	1.90	0.54
1:C:199:GLU:CB	1:H:216:GLU:CG	2.75	0.54
1:G:36:VAL:HB	1:G:62:PHE:CE2	2.43	0.54
1:G:127:ILE:HG22	1:G:223:GLN:HE21	1.73	0.53
1:C:74:ALA:HA	2:C:301:CL:CL	2.45	0.53
1:F:99:ARG:C	1:F:99:ARG:CD	2.76	0.53
1:A:215:LEU:HD22	1:C:71:CYS:SG	2.49	0.53
1:E:36:VAL:HB	1:E:62:PHE:CE1	2.44	0.53
1:E:123:GLN:NE2	1:E:196:LEU:HD12	2.23	0.53
1:F:197:ASN:HB2	1:F:200:ARG:HD3	1.91	0.53
1:G:186:SER:HB3	1:H:186:SER:O	2.09	0.53
1:A:72:ASN:ND2	3:A:402:HOH:O	2.41	0.52
1:F:29:SER:O	1:F:55:GLN:HG2	2.09	0.52
1:C:36:VAL:HB	1:C:62:PHE:CE2	2.44	0.52
1:C:199:GLU:HG2	1:H:216:GLU:HB2	1.87	0.52
1:A:210:VAL:HG23	1:A:215:LEU:HD23	1.91	0.51
1:E:210:VAL:HG23	1:E:215:LEU:HD23	1.93	0.51
1:D:215:LEU:HD22	1:E:71:CYS:SG	2.51	0.51
1:C:198:PRO:CD	1:C:199:GLU:OE1	2.58	0.51
1:B:96:ILE:CG2	1:B:100:ALA:HB3	2.41	0.51
1:D:99:ARG:HA	1:F:202:PHE:HB3	1.92	0.50
1:D:36:VAL:HB	1:D:62:PHE:CE2	2.47	0.50
1:E:215:LEU:HD22	1:F:71:CYS:SG	2.52	0.50
1:G:127:ILE:HG22	1:G:223:GLN:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:VAL:HB	1:H:62:PHE:CE2	2.47	0.50
1:C:93:MET:HG3	1:E:211:LYS:HE3	1.94	0.50
1:D:130:CYS:SG	1:D:223:GLN:OE1	2.70	0.50
1:B:201:MET:HG2	1:B:202:PHE:CD2	2.47	0.49
1:G:57:PHE:CE1	1:G:105:ILE:HG12	2.47	0.49
1:A:99:ARG:HA	1:B:202:PHE:HB3	1.94	0.49
1:C:199:GLU:OE1	1:C:199:GLU:N	2.46	0.49
1:F:99:ARG:HD2	1:F:100:ALA:N	2.27	0.49
1:D:203:ARG:HH11	1:E:99:ARG:NH1	2.09	0.49
1:F:36:VAL:HB	1:F:62:PHE:CE1	2.47	0.49
1:B:118:ILE:HG12	1:B:134:TRP:CZ3	2.47	0.49
1:H:197:ASN:HB3	1:H:200:ARG:HB2	1.95	0.49
1:A:36:VAL:HB	1:A:62:PHE:CE1	2.47	0.49
1:B:210:VAL:HG13	1:B:215:LEU:HD23	1.94	0.48
1:H:74:ALA:HA	2:H:301:CL:CL	2.49	0.48
1:C:199:GLU:HB3	1:H:216:GLU:CG	2.42	0.48
1:B:99:ARG:HB3	1:H:88:LEU:HD12	1.95	0.48
1:A:186:SER:O	1:F:186:SER:HB3	2.14	0.47
1:H:6:PHE:CD1	1:H:116:ILE:HG12	2.49	0.47
1:D:177:HIS:HD2	1:D:181:THR:OG1	1.97	0.47
1:D:227:LYS:CE	3:D:401:HOH:O	2.62	0.47
1:F:89:MET:CE	3:F:404:HOH:O	2.62	0.47
1:E:218:ILE:HD12	1:F:63:LEU:HD22	1.96	0.47
1:B:71:CYS:SG	1:C:215:LEU:HD22	2.55	0.47
1:D:218:ILE:HD12	1:E:63:LEU:HD22	1.96	0.47
1:E:41:ARG:HH21	1:F:41:ARG:NH1	2.12	0.47
1:F:99:ARG:CZ	1:F:100:ALA:HA	2.45	0.47
1:C:102:GLU:HB3	1:C:103:PRO:HD3	1.97	0.47
1:E:152:GLU:CD	1:F:41:ARG:HH12	2.18	0.47
1:D:71:CYS:SG	1:F:215:LEU:HD22	2.55	0.47
1:G:102:GLU:HB3	1:G:103:PRO:HD3	1.97	0.47
1:B:36:VAL:HB	1:B:62:PHE:CE1	2.50	0.47
1:D:227:LYS:HE2	3:D:401:HOH:O	2.14	0.47
1:F:200:ARG:HH12	1:F:206:ILE:HG13	1.80	0.47
1:G:177:HIS:HD2	1:G:181:THR:OG1	1.98	0.47
1:A:64:PHE:HB3	1:B:191:PHE:CE2	2.51	0.46
1:B:99:ARG:C	1:B:101:LEU:N	2.67	0.46
1:A:99:ARG:HE	1:B:203:ARG:HH12	1.62	0.46
1:A:228:LYS:HE2	1:A:228:LYS:HB3	1.79	0.46
1:C:200:ARG:HH22	1:H:216:GLU:HG2	1.81	0.46
1:H:227:LYS:HD2	1:H:227:LYS:HA	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:ASP:HB3	1:G:49:THR:CG2	2.45	0.46
1:B:40:GLN:HE22	1:E:37:GLN:NE2	2.08	0.45
1:B:181:THR:HG21	3:B:431:HOH:O	2.16	0.45
1:G:200:ARG:O	1:G:200:ARG:HG2	2.16	0.45
1:C:197:ASN:HA	1:C:198:PRO:HD3	1.60	0.45
1:D:104:TYR:HB3	1:D:174:LEU:HD11	1.99	0.45
1:B:186:SER:HB3	1:D:186:SER:O	2.16	0.45
1:D:201:MET:O	1:D:202:PHE:HB2	2.17	0.45
1:G:178:GLY:HA3	2:G:301:CL:CL	2.54	0.45
1:G:200:ARG:O	1:G:200:ARG:CG	2.64	0.45
3:E:429:HOH:O	1:F:43:HIS:HE1	1.98	0.44
1:H:197:ASN:HA	1:H:198:PRO:HD3	1.85	0.44
1:D:41:ARG:HA	1:D:41:ARG:HD2	1.52	0.44
1:G:104:TYR:HB3	1:G:174:LEU:HD11	1.99	0.44
1:B:56:ARG:CZ	1:C:198:PRO:HA	2.47	0.44
1:G:90:PRO:HB2	3:G:401:HOH:O	2.16	0.44
1:E:104:TYR:HB3	1:E:174:LEU:HD11	1.98	0.44
1:F:177:HIS:HD2	1:F:181:THR:OG1	2.01	0.44
1:H:96:ILE:CG1	1:H:101:LEU:HD23	2.47	0.44
1:D:6:PHE:CD1	1:D:116:ILE:HG12	2.53	0.44
1:A:218:ILE:HD12	1:C:63:LEU:HD22	1.99	0.44
1:C:6:PHE:CD1	1:C:116:ILE:HG12	2.53	0.44
1:D:35:PHE:HB2	1:D:43:HIS:O	2.17	0.44
1:G:200:ARG:HG3	1:G:203:ARG:HB2	2.00	0.44
1:A:202:PHE:CB	1:C:99:ARG:HG3	2.47	0.43
1:D:203:ARG:NH1	1:E:99:ARG:NH1	2.66	0.43
1:E:41:ARG:NH2	1:F:41:ARG:NH1	2.66	0.43
1:H:55:GLN:HE21	1:H:55:GLN:HB3	1.56	0.43
1:H:130:CYS:SG	1:H:223:GLN:NE2	2.91	0.43
1:D:138:TRP:CD1	1:D:166:GLU:HG2	2.53	0.43
1:A:77:ASN:HB3	1:D:77:ASN:HB3	2.01	0.43
1:F:89:MET:HE2	3:F:404:HOH:O	2.18	0.43
1:C:186:SER:O	1:E:186:SER:HB3	2.18	0.43
1:E:177:HIS:HD2	1:E:181:THR:OG1	2.02	0.43
1:E:59:THR:HG23	3:E:421:HOH:O	2.20	0.42
1:F:104:TYR:HB3	1:F:174:LEU:HD11	2.00	0.42
1:F:6:PHE:CD1	1:F:116:ILE:HG12	2.54	0.42
1:B:104:TYR:HB3	1:B:174:LEU:HD11	2.01	0.42
1:H:96:ILE:CG1	1:H:101:LEU:CD2	2.97	0.42
1:H:205:PRO:O	1:H:207:PRO:HD3	2.20	0.42
1:D:200:ARG:HA	1:D:203:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:ARG:NH2	3:E:402:HOH:O	2.52	0.42
1:F:118:ILE:HG12	1:F:134:TRP:CZ3	2.54	0.42
1:G:197:ASN:HA	1:G:198:PRO:HD3	1.90	0.42
1:H:134:TRP:CD1	1:H:227:LYS:HD3	2.55	0.42
1:H:134:TRP:CZ2	1:H:227:LYS:HG2	2.54	0.42
1:H:204:LYS:O	1:H:204:LYS:HD3	2.20	0.42
1:H:25:VAL:HA	1:H:26:PRO:HD3	1.94	0.42
1:B:47:LEU:HA	1:B:52:SER:CB	2.50	0.41
1:F:89:MET:HE2	1:F:183:ASN:OD1	2.19	0.41
1:A:74:ALA:HA	2:A:301:CL:CL	2.57	0.41
1:D:47:LEU:HA	1:D:52:SER:CB	2.50	0.41
1:H:131:PRO:HG2	1:H:134:TRP:CD1	2.55	0.41
1:A:99:ARG:NH2	1:B:203:ARG:NH2	2.68	0.41
1:D:25:VAL:HA	1:D:26:PRO:HD3	1.93	0.41
1:F:200:ARG:HH12	1:F:206:ILE:CG1	2.33	0.41
1:H:214:GLU:HB3	1:H:217:LYS:HD2	2.02	0.41
1:F:29:SER:O	1:F:55:GLN:CG	2.68	0.41
1:C:25:VAL:HA	1:C:26:PRO:HD3	1.91	0.41
1:C:118:ILE:HG12	1:C:134:TRP:CZ3	2.56	0.41
1:E:118:ILE:HG12	1:E:134:TRP:CZ3	2.56	0.41
1:G:122:SER:O	1:G:123:GLN:HB2	2.21	0.41
1:D:64:PHE:HB3	1:F:191:PHE:CE2	2.56	0.41
1:G:128:PRO:HA	1:G:129:PRO:HD3	1.99	0.41
1:C:107:ARG:HE	1:C:107:ARG:HB3	1.40	0.40
1:C:199:GLU:CB	1:H:216:GLU:CD	2.89	0.40
1:C:200:ARG:NH2	1:H:215:LEU:HB2	2.36	0.40
1:D:74:ALA:HA	2:D:301:CL:CL	2.58	0.40
1:E:123:GLN:NE2	1:E:196:LEU:CD1	2.84	0.40
1:C:41:ARG:NH2	1:C:152:GLU:OE1	2.53	0.40
1:D:56:ARG:HB2	1:F:123:GLN:NE2	2.37	0.40
1:C:199:GLU:HB3	1:H:216:GLU:HG3	1.91	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:GLU:OE1	1:G:199:GLU:CG[2_455]	2.04	0.16



## 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	223/230 (97%)	216 (97%)	7 (3%)	0	100	100
1	B	225/230 (98%)	216 (96%)	9 (4%)	0	100	100
1	C	223/230 (97%)	215 (96%)	8 (4%)	0	100	100
1	D	225/230 (98%)	217 (96%)	8 (4%)	0	100	100
1	E	223/230 (97%)	217 (97%)	6 (3%)	0	100	100
1	F	224/230 (97%)	217 (97%)	7 (3%)	0	100	100
1	G	223/230 (97%)	215 (96%)	8 (4%)	0	100	100
1	H	223/230 (97%)	216 (97%)	7 (3%)	0	100	100
All	All	1789/1840 (97%)	1729 (97%)	60 (3%)	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 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	191/197 (97%)	183 (96%)	8 (4%)	30	58
1	B	192/197 (98%)	186 (97%)	6 (3%)	40	69
1	C	190/197 (96%)	183 (96%)	7 (4%)	34	63
1	D	192/197 (98%)	186 (97%)	6 (3%)	40	69
1	E	190/197 (96%)	182 (96%)	8 (4%)	30	58
1	F	191/197 (97%)	186 (97%)	5 (3%)	46	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	190/197 (96%)	178 (94%)	12 (6%)	18	40
1	H	190/197 (96%)	179 (94%)	11 (6%)	20	43
All	All	1526/1576 (97%)	1463 (96%)	63 (4%)	30	59

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	56	ARG
1	A	91	MET
1	A	97	THR
1	A	99	ARG
1	A	102	GLU
1	A	116	ILE
1	A	228	LYS
1	B	41	ARG
1	B	91[A]	MET
1	B	91[B]	MET
1	B	97	THR
1	B	203	ARG
1	B	210	VAL
1	C	41	ARG
1	C	55	GLN
1	C	56	ARG
1	C	97	THR
1	C	99	ARG
1	C	107	ARG
1	C	203	ARG
1	D	4	ARG
1	D	41	ARG
1	D	88	LEU
1	D	97	THR
1	D	201	MET
1	D	223	GLN
1	E	41	ARG
1	E	97	THR
1	E	99	ARG
1	E	172	PRO
1	E	199	GLU
1	E	200	ARG
1	E	203	ARG

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Mol	Chain	Res	Type
1	E	206	ILE
1	F	41	ARG
1	F	97	THR
1	F	99	ARG
1	F	200	ARG
1	F	211	LYS
1	G	22	GLU
1	G	41	ARG
1	G	49	THR
1	G	56	ARG
1	G	69	ASP
1	G	91	MET
1	G	97	THR
1	G	99	ARG
1	G	139	LYS
1	G	199	GLU
1	G	203	ARG
1	G	216	GLU
1	H	41	ARG
1	H	55	GLN
1	H	97	THR
1	H	99	ARG
1	H	199	GLU
1	H	200	ARG
1	H	201	MET
1	H	204	LYS
1	H	214	GLU
1	H	217	LYS
1	H	227	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	72	ASN
1	A	223	GLN
1	B	223	GLN
1	C	55	GLN
1	C	223	GLN
1	D	37	GLN
1	D	72	ASN
1	D	177	HIS

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Mol	Chain	Res	Type
1	E	37	GLN
1	E	77	ASN
1	E	123	GLN
1	E	177	HIS
1	F	177	HIS
1	G	40	GLN
1	G	72	ASN
1	G	177	HIS
1	G	223	GLN
1	H	40	GLN
1	H	55	GLN
1	H	223	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	225/230 (97%)	-0.60	0 100 100	4, 25, 44, 49	0
1	B	226/230 (98%)	-0.67	0 100 100	4, 24, 42, 48	0
1	C	225/230 (97%)	-0.50	0 100 100	7, 28, 49, 53	0
1	D	227/230 (98%)	-0.59	0 100 100	5, 25, 47, 55	0
1	E	225/230 (97%)	-0.59	0 100 100	8, 28, 44, 49	0
1	F	226/230 (98%)	-0.60	0 100 100	6, 25, 43, 46	0
1	G	225/230 (97%)	-0.56	0 100 100	6, 27, 43, 48	0
1	H	225/230 (97%)	-0.64	0 100 100	5, 26, 40, 44	0
All	All	1804/1840 (98%)	-0.59	0 100 100	4, 26, 44, 55	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CL	F	301	1/1	0.94	0.10	27,27,27,27	0
2	CL	B	303	1/1	0.96	0.09	27,27,27,27	0
2	CL	G	303	1/1	0.96	0.19	27,27,27,27	0
2	CL	F	302	1/1	0.97	0.07	27,27,27,27	0
2	CL	E	301	1/1	0.97	0.17	27,27,27,27	0
2	CL	H	301	1/1	0.97	0.06	26,26,26,26	0
2	CL	C	301	1/1	0.98	0.09	26,26,26,26	0
2	CL	A	302	1/1	0.98	0.09	27,27,27,27	0
2	CL	A	303	1/1	0.98	0.06	26,26,26,26	0
2	CL	B	301	1/1	0.98	0.08	25,25,25,25	0
2	CL	G	302	1/1	0.98	0.10	25,25,25,25	0
2	CL	B	302	1/1	0.98	0.12	27,27,27,27	0
2	CL	A	301	1/1	0.98	0.10	27,27,27,27	0
2	CL	D	301	1/1	0.99	0.17	27,27,27,27	0
2	CL	C	302	1/1	0.99	0.07	27,27,27,27	0
2	CL	G	301	1/1	0.99	0.12	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.