



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2021 – 10:51 AM EST

PDB ID : 7SFX  
Title : 10A1 Fab in complex with CD99 peptide  
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Deposited on : 2021-10-04  
Resolution : 3.10 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.

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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	:	2.25
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)	:	2.25

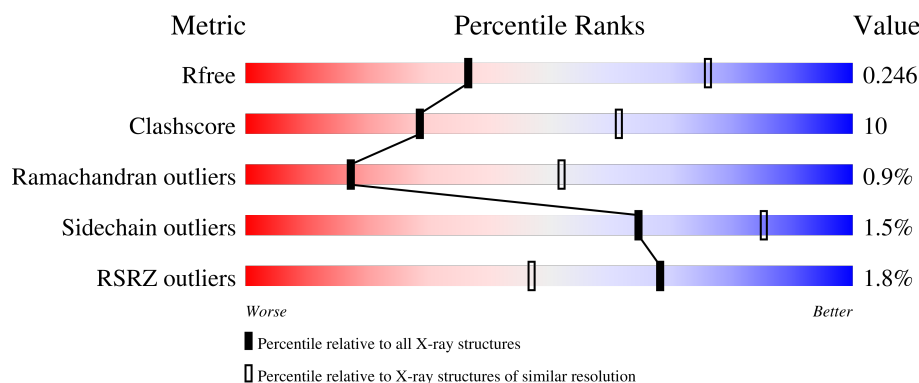
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	247	<div> <div>0%</div> <div>72%</div> <div>17%</div> <div>11%</div> </div>
1	C	247	<div> <div>71%</div> <div>19%</div> <div>11%</div> </div>
1	G	247	<div> <div>69%</div> <div>19%</div> <div>11%</div> </div>
1	J	247	<div> <div>4%</div> <div>68%</div> <div>17%</div> <div>14%</div> </div>
2	B	215	<div> <div>2%</div> <div>82%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	215	<div><div></div><div>86%14%</div></div>
2	H	215	<div><div></div><div>73%24%</div><div></div></div>
2	K	215	<div><div></div><div>4%70%23%6%</div></div>
3	E	14	<div><div></div><div>14%21%29%50%</div></div>
3	F	14	<div><div></div><div>29%21%50%</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25893 atoms, of which 12755 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 10A1 Fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	221	Total	C	H	N	O	S	0	0	0
			3286	1046	1626	280	329	5			
1	A	221	Total	C	H	N	O	S	0	0	0
			3286	1046	1626	280	329	5			
1	G	219	Total	C	H	N	O	S	0	0	0
			3262	1039	1615	278	325	5			
1	J	213	Total	C	H	N	O	S	0	0	0
			3206	1023	1590	270	319	4			

- Molecule 2 is a protein called 10A1 Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	214	Total	C	H	N	O	S	0	0	0
			3185	1015	1560	271	335	4			
2	B	214	Total	C	H	N	O	S	0	0	0
			3185	1015	1560	271	335	4			
2	H	214	Total	C	H	N	O	S	0	0	0
			3185	1015	1560	271	335	4			
2	K	203	Total	C	H	N	O	S	0	0	0
			3070	983	1506	260	317	4			

- Molecule 3 is a protein called CD99 antigen peptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	7	Total	C	H	N	O	S	0	0	0
			109	35	56	9	8	1			
3	E	7	Total	C	H	N	O	S	0	0	0
			109	35	56	9	8	1			

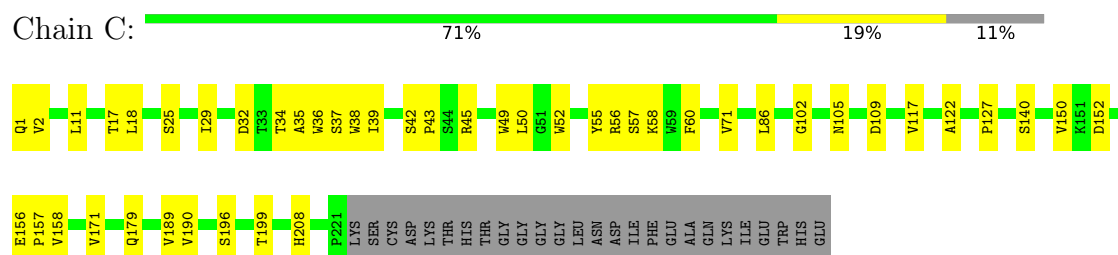
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	O 2	0	0
4	F	1	Total 1	O 1	0	0
4	A	1	Total 1	O 1	0	0
4	B	1	Total 1	O 1	0	0
4	E	1	Total 1	O 1	0	0
4	H	3	Total 3	O 3	0	0
4	J	1	Total 1	O 1	0	0

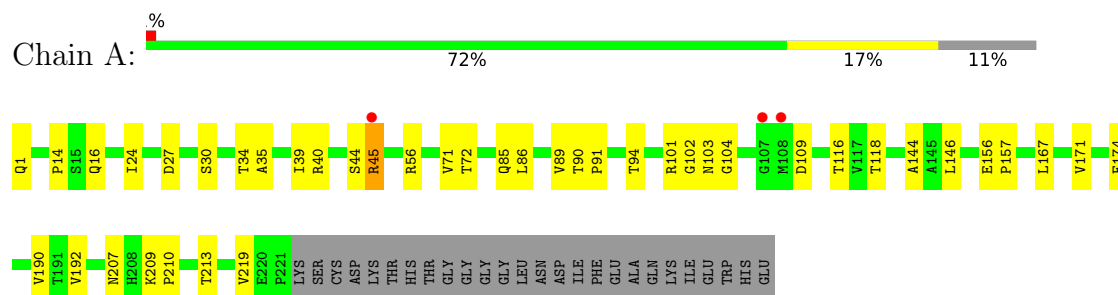
### 3 Residue-property plots [i](#)

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.

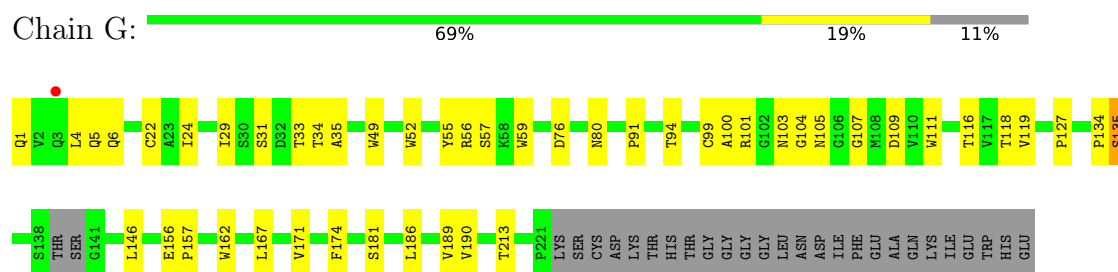
#### • Molecule 1: 10A1 Fab heavy chain



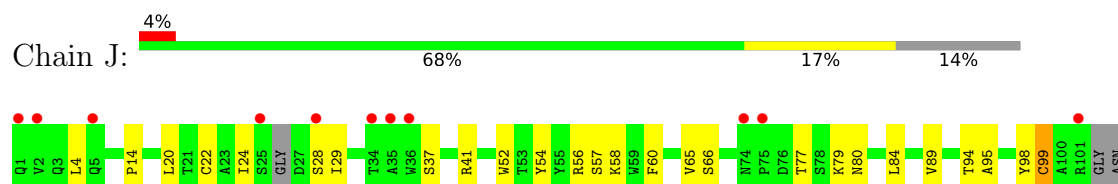
#### • Molecule 1: 10A1 Fab heavy chain

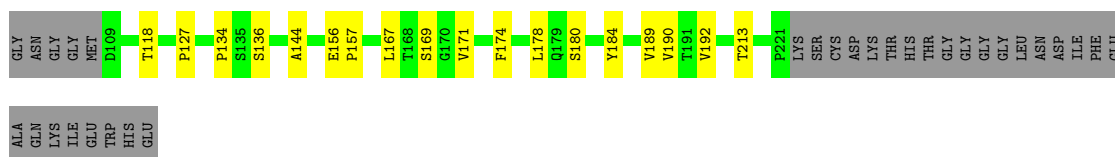


#### • Molecule 1: 10A1 Fab heavy chain



#### • Molecule 1: 10A1 Fab heavy chain





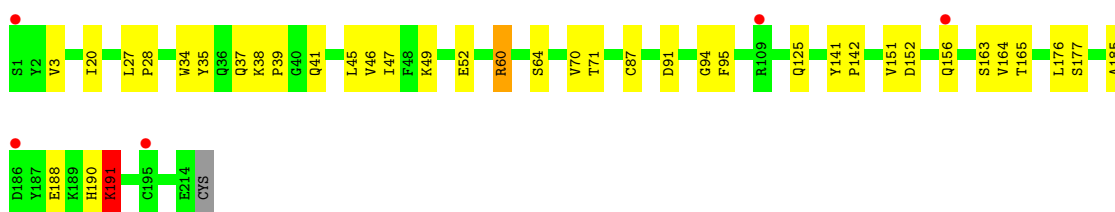
- Molecule 2: 10A1 Fab light chain

Chain D: 86% 14%



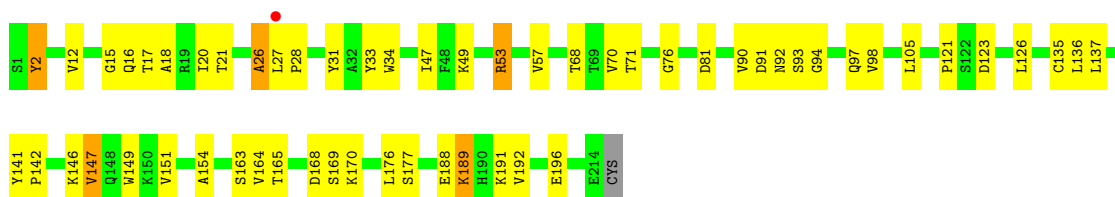
- Molecule 2: 10A1 Fab light chain

Chain B: 2% 82% 17%



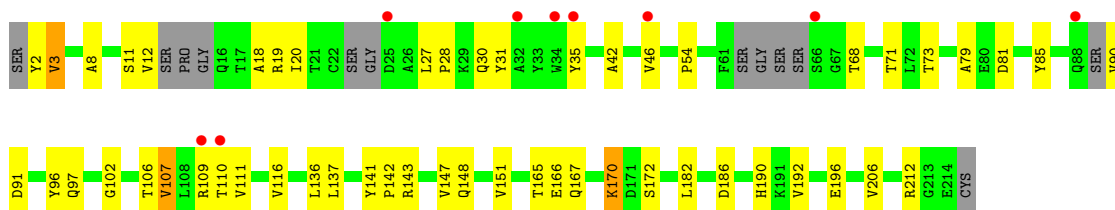
- Molecule 2: 10A1 Fab light chain

Chain H: 73% 24%



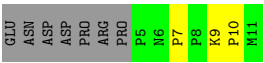
- Molecule 2: 10A1 Fab light chain

Chain K: 4% 70% 23% 6%

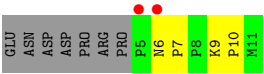


- Molecule 3: CD99 antigen peptide

Chain F: 29% 21% 50%



● Molecule 3: CD99 antigen peptide





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.41Å 131.55Å 119.81Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	46.38 – 3.10 46.38 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.38-3.10) 97.4 (46.38-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.226 , 0.248 0.226 , 0.246	Depositor DCC
$R_{free}$ test set	1847 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 8.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.347 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	25893	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<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](#)

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	0.31	0/1703	0.60	0/2330
1	C	0.32	0/1703	0.61	0/2330
1	G	0.31	0/1689	0.59	0/2309
1	J	0.41	0/1657	0.66	0/2267
2	B	0.30	0/1661	0.61	0/2261
2	D	0.35	0/1661	0.62	0/2261
2	H	0.37	0/1661	0.63	0/2261
2	K	0.33	0/1595	0.61	0/2166
3	E	0.32	0/56	0.54	0/76
3	F	0.35	0/56	0.46	0/76
All	All	0.34	0/13442	0.62	0/18337

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	1660	1626	1626	31	0
1	C	1660	1626	1626	28	0
1	G	1647	1615	1613	45	0
1	J	1616	1590	1588	28	0
2	B	1625	1560	1560	28	0
2	D	1625	1560	1560	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1625	1560	1560	45	0
2	K	1564	1506	1502	37	0
3	E	53	56	56	7	0
3	F	53	56	56	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	H	3	0	0	0	0
4	J	1	0	0	0	0
All	All	13138	12755	12747	251	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 10.

All (251) 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)
3:E:6:ASN:HB2	3:E:7:PRO:HD2	1.36	1.06
2:D:93:SER:O	3:F:7:PRO:HG3	1.76	0.86
1:J:24:ILE:HD12	1:J:24:ILE:O	1.79	0.82
1:G:4:LEU:HD21	1:G:99:CYS:SG	2.19	0.82
1:G:107:GLY:HA2	2:H:33:TYR:HE2	1.45	0.81
2:B:95:PHE:CE2	3:E:7:PRO:HD3	2.16	0.80
1:G:31:SER:OG	1:G:34:THR:HB	1.82	0.80
3:E:6:ASN:CB	3:E:7:PRO:HD2	2.12	0.79
1:G:34:THR:OG1	1:G:103:ASN:HB2	1.86	0.76
2:K:2:TYR:O	2:K:3:VAL:HG12	1.87	0.75
1:C:38:TRP:O	1:C:39:ILE:HD13	1.88	0.73
3:F:9:LYS:HG3	3:F:10:PRO:HD2	1.70	0.73
1:C:152:ASP:OD1	1:C:179:GLN:NE2	2.25	0.70
2:B:151:VAL:HG23	2:B:152:ASP:H	1.58	0.69
2:K:90:VAL:HG12	2:K:91:ASP:H	1.58	0.68
1:G:34:THR:HG23	1:G:103:ASN:HB2	1.74	0.68
1:J:171:VAL:HG22	1:J:190:VAL:HG12	1.75	0.68
1:A:171:VAL:HG22	1:A:190:VAL:HG12	1.74	0.68
2:K:111:VAL:HG12	2:K:111:VAL:O	1.94	0.68
2:B:141:TYR:HB3	2:B:142:PRO:HD3	1.78	0.66
1:C:109:ASP:HB3	1:G:1:GLN:HE22	1.61	0.65
1:A:34:THR:HG23	1:A:34:THR:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:GLN:NE2	2:B:41:GLN:O	2.29	0.65
1:G:31:SER:CB	1:G:34:THR:HB	2.26	0.64
2:H:2:TYR:CE1	2:H:98:VAL:HG11	2.32	0.64
1:G:29:ILE:HB	1:G:80:ASN:OD1	1.97	0.64
1:G:34:THR:CB	1:G:103:ASN:HB2	2.27	0.64
1:G:34:THR:CG2	1:G:103:ASN:HB2	2.28	0.64
1:C:32:ASP:C	1:C:34:THR:HG23	2.18	0.64
2:K:141:TYR:HB3	2:K:142:PRO:HD3	1.80	0.63
2:B:60:ARG:H	2:B:60:ARG:HD2	1.62	0.63
2:H:168:ASP:O	2:H:169:SER:OG	2.15	0.62
2:H:26:ALA:HB1	2:H:28:PRO:HD3	1.80	0.62
2:D:141:TYR:HB3	2:D:142:PRO:HD3	1.82	0.62
1:G:174:PHE:CD2	2:H:165:THR:HG23	2.35	0.61
2:B:64:SER:O	2:B:70:VAL:HG13	2.01	0.61
2:B:38:LYS:HB3	2:B:39:PRO:HD2	1.82	0.61
2:D:163:SER:O	2:D:176:LEU:HD12	2.00	0.60
2:H:141:TYR:HB3	2:H:142:PRO:HD3	1.83	0.59
2:H:49:LYS:HG2	2:H:49:LYS:O	2.01	0.59
3:E:9:LYS:HG2	3:E:10:PRO:HD2	1.84	0.59
2:B:151:VAL:HG13	2:B:156:GLN:CD	2.23	0.58
1:G:107:GLY:HA2	2:H:33:TYR:CE2	2.31	0.58
2:B:91:ASP:O	2:B:94:GLY:N	2.36	0.58
1:J:94:THR:HG23	1:J:118:THR:HA	1.86	0.57
1:A:72:THR:HG23	1:A:85:GLN:HB2	1.87	0.56
2:H:2:TYR:CD1	2:H:98:VAL:HG11	2.40	0.56
1:C:32:ASP:O	1:C:34:THR:HG23	2.06	0.56
2:B:34:TRP:O	2:B:45:LEU:HD12	2.06	0.55
1:C:189:VAL:HG21	2:D:136:LEU:HD22	1.89	0.55
1:C:171:VAL:HG22	1:C:190:VAL:HG12	1.89	0.55
1:A:207:ASN:ND2	1:A:213:THR:O	2.41	0.54
2:H:12:VAL:HG21	2:H:18:ALA:CB	2.38	0.54
2:H:121:PRO:HB2	2:H:126:LEU:HD11	1.88	0.54
1:G:94:THR:HG23	1:G:118:THR:HA	1.88	0.54
2:K:170:LYS:C	2:K:172:SER:H	2.11	0.54
1:C:2:VAL:O	1:C:2:VAL:HG13	2.07	0.54
2:H:16:GLN:HG2	2:H:76:GLY:HA2	1.89	0.53
1:G:35:ALA:HB1	1:G:52:TRP:HE1	1.73	0.53
1:G:24:ILE:HD11	1:G:80:ASN:CG	2.29	0.53
2:H:16:GLN:C	2:H:17:THR:HG22	2.29	0.53
1:G:31:SER:HB2	1:G:34:THR:HB	1.91	0.53
2:H:27:LEU:N	2:H:28:PRO:HD3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:LYS:HB2	2:B:52:GLU:HG3	1.91	0.52
2:D:151:VAL:HG23	2:D:152:ASP:N	2.24	0.52
2:K:151:VAL:O	2:K:192:VAL:O	2.28	0.52
2:B:163:SER:O	2:B:176:LEU:HD12	2.09	0.52
3:E:6:ASN:O	3:E:7:PRO:C	2.48	0.52
1:J:144:ALA:HB3	1:J:192:VAL:O	2.10	0.52
1:C:196:SER:HA	1:C:199:THR:HG22	1.90	0.52
2:H:151:VAL:HG23	2:H:154:ALA:HB3	1.91	0.52
2:K:90:VAL:HG12	2:K:91:ASP:N	2.23	0.52
2:B:3:VAL:HG21	2:K:8:ALA:HB3	1.92	0.51
2:K:18:ALA:O	2:K:73:THR:HA	2.10	0.51
2:D:107:VAL:O	2:D:109:ARG:HG3	2.10	0.51
1:A:44:SER:O	1:A:45:ARG:CB	2.57	0.51
1:J:41:ARG:O	1:J:95:ALA:HB1	2.11	0.51
2:D:162:GLU:HB3	2:D:176:LEU:HD11	1.91	0.51
2:H:146:LYS:O	2:H:147:VAL:HG12	2.10	0.51
1:A:34:THR:HG22	1:A:102:GLY:O	2.10	0.51
1:A:144:ALA:HB3	1:A:192:VAL:HG23	1.92	0.51
2:B:190:HIS:O	2:B:191:LYS:CB	2.59	0.51
1:G:33:THR:HG23	1:G:33:THR:O	2.11	0.51
2:K:20:ILE:O	2:K:71:THR:HG23	2.10	0.51
2:B:141:TYR:HB3	2:B:142:PRO:CD	2.39	0.51
2:K:190:HIS:O	2:K:212:ARG:NH1	2.44	0.51
1:G:100:ALA:HB2	1:G:111:TRP:CE3	2.46	0.50
2:H:146:LYS:O	2:H:147:VAL:O	2.28	0.50
3:E:6:ASN:HB2	3:E:7:PRO:CD	2.25	0.50
2:K:91:ASP:N	2:K:96:TYR:O	2.43	0.50
1:A:156:GLU:N	1:A:157:PRO:HD3	2.26	0.50
1:A:209:LYS:N	1:A:210:PRO:HD2	2.26	0.50
2:H:151:VAL:O	2:H:154:ALA:N	2.44	0.50
2:B:95:PHE:CZ	3:E:7:PRO:HD3	2.45	0.50
2:H:91:ASP:O	2:H:94:GLY:N	2.43	0.50
1:J:4:LEU:HD22	1:J:99:CYS:SG	2.52	0.50
1:A:34:THR:O	1:A:34:THR:CG2	2.60	0.50
2:K:90:VAL:HA	2:K:97:GLN:HA	1.92	0.50
2:K:106:THR:O	2:K:107:VAL:O	2.30	0.50
2:K:27:LEU:N	2:K:28:PRO:CD	2.75	0.50
1:G:189:VAL:HG21	2:H:136:LEU:HD13	1.93	0.49
1:A:109:ASP:OD2	2:B:35:TYR:OH	2.22	0.49
1:G:174:PHE:HA	2:H:165:THR:HG22	1.94	0.49
1:J:54:TYR:HB2	1:J:60:PHE:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:SER:OG	1:C:43:PRO:HD2	2.13	0.49
1:G:174:PHE:CE2	2:H:165:THR:HG23	2.47	0.49
2:H:163:SER:O	2:H:176:LEU:HD12	2.13	0.49
1:C:1:GLN:OE1	1:G:5:GLN:NE2	2.46	0.49
2:D:187:TYR:O	2:D:193:TYR:OH	2.29	0.49
2:H:53:ARG:HE	2:H:57:VAL:HG23	1.78	0.49
1:G:49:TRP:CE3	2:H:97:GLN:O	2.67	0.48
1:J:171:VAL:HG22	1:J:190:VAL:CG1	2.40	0.48
2:D:151:VAL:O	2:D:192:VAL:O	2.32	0.48
1:A:71:VAL:HG12	1:A:86:LEU:HD13	1.96	0.48
1:A:101:ARG:O	1:A:109:ASP:HA	2.13	0.48
2:B:164:VAL:HG23	2:B:176:LEU:HD13	1.95	0.48
2:B:20:ILE:O	2:B:71:THR:OG1	2.26	0.48
1:G:174:PHE:O	1:G:186:LEU:HD11	2.14	0.48
1:A:30:SER:HB3	1:A:56:ARG:HB2	1.96	0.48
2:H:137:LEU:N	2:H:137:LEU:HD12	2.29	0.47
2:B:164:VAL:CG2	2:B:176:LEU:HD13	2.45	0.47
1:J:98:TYR:CE1	2:K:42:ALA:HB2	2.49	0.47
2:D:119:PHE:HB2	2:D:134:VAL:HB	1.95	0.47
2:B:60:ARG:HD2	2:B:60:ARG:N	2.29	0.47
2:B:176:LEU:HD12	2:B:177:SER:H	1.78	0.47
1:G:34:THR:O	1:G:35:ALA:HB3	2.15	0.47
2:K:46:VAL:O	2:K:54:PRO:HG2	2.15	0.47
2:K:107:VAL:O	2:K:107:VAL:HG13	2.15	0.47
2:K:109:ARG:O	2:K:109:ARG:CG	2.63	0.47
2:K:110:THR:HB	2:K:141:TYR:HB2	1.97	0.47
1:G:34:THR:HG23	1:G:103:ASN:CB	2.44	0.47
2:H:12:VAL:HG21	2:H:18:ALA:HB2	1.97	0.46
1:A:34:THR:HG22	1:A:103:ASN:O	2.16	0.46
1:G:171:VAL:HG22	1:G:190:VAL:HG12	1.97	0.46
2:D:111:VAL:HG13	2:D:111:VAL:O	2.14	0.46
2:B:190:HIS:O	2:B:191:LYS:HB2	2.15	0.46
2:H:70:VAL:HG12	2:H:71:THR:N	2.31	0.46
2:K:19:ARG:HB2	2:K:19:ARG:NH1	2.31	0.46
2:K:116:VAL:HG21	2:K:206:VAL:HG13	1.98	0.46
2:H:191:LYS:CG	2:H:192:VAL:N	2.79	0.46
1:C:2:VAL:HA	1:C:25:SER:O	2.16	0.46
1:G:91:PRO:HA	1:G:119:VAL:HB	1.96	0.46
1:C:109:ASP:HB3	1:G:1:GLN:NE2	2.29	0.45
1:A:39:ILE:HG22	1:A:40:ARG:N	2.31	0.45
1:G:56:ARG:O	1:G:57:SER:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:GLN:HG2	1:G:99:CYS:SG	2.57	0.45
1:A:24:ILE:HD12	1:A:27:ASP:O	2.16	0.45
1:C:35:ALA:HB3	1:C:102:GLY:H	1.81	0.45
2:K:182:LEU:HG	2:K:186:ASP:HB2	1.99	0.45
2:D:164:VAL:HG22	2:D:176:LEU:HD13	1.99	0.45
1:J:29:ILE:O	1:J:29:ILE:HG23	2.17	0.45
2:D:79:ALA:HA	2:D:107:VAL:HG11	1.99	0.45
1:A:146:LEU:HD12	1:A:219:VAL:CG2	2.47	0.45
1:A:94:THR:HG23	1:A:118:THR:HA	1.99	0.45
1:A:16:GLN:O	1:A:89:VAL:HG23	2.17	0.44
2:D:111:VAL:HG23	2:D:142:PRO:HG2	1.99	0.44
1:G:4:LEU:HD12	1:G:24:ILE:HG22	1.99	0.44
2:H:20:ILE:HG22	2:H:21:THR:N	2.32	0.44
2:H:92:ASN:O	2:H:93:SER:OG	2.32	0.44
1:J:189:VAL:HG11	2:K:136:LEU:HD22	1.98	0.44
1:A:101:ARG:HG2	1:A:102:GLY:N	2.32	0.44
2:B:27:LEU:N	2:B:28:PRO:HD2	2.32	0.44
1:C:37:SER:HG	1:C:52:TRP:HD1	1.64	0.44
1:C:156:GLU:N	1:C:157:PRO:HD3	2.33	0.44
1:J:167:LEU:O	1:J:169:SER:N	2.49	0.44
1:C:56:ARG:O	1:C:57:SER:C	2.55	0.44
1:J:65:VAL:HG13	1:J:66:SER:N	2.32	0.44
1:C:49:TRP:C	1:C:50:LEU:HD12	2.38	0.44
2:D:105:LEU:HG	2:D:107:VAL:HG23	2.00	0.44
1:G:104:GLY:O	1:G:105:ASN:HB3	2.17	0.44
1:G:116:THR:HB	1:G:157:PRO:HG3	2.00	0.44
2:H:34:TRP:HB2	2:H:47:ILE:HB	2.00	0.44
1:J:28:SER:O	1:J:29:ILE:HG22	2.17	0.44
1:C:58:LYS:O	1:C:60:PHE:CD1	2.70	0.44
1:A:34:THR:HG22	1:A:102:GLY:C	2.38	0.44
1:A:44:SER:O	1:A:45:ARG:HB2	2.17	0.44
1:G:134:PRO:O	1:G:135:SER:CB	2.65	0.44
1:G:189:VAL:HG11	2:H:136:LEU:HD22	2.00	0.44
2:K:27:LEU:HB2	2:K:68:THR:HA	2.00	0.44
1:G:55:TYR:O	1:G:59:TRP:HA	2.18	0.43
2:K:79:ALA:HB1	2:K:172:SER:HB3	2.00	0.43
2:D:35:TYR:CE1	2:D:88:GLN:OE1	2.71	0.43
1:A:167:LEU:O	1:A:171:VAL:HG23	2.17	0.43
2:B:185:ALA:O	2:B:188:GLU:HG2	2.18	0.43
1:A:144:ALA:HB3	1:A:192:VAL:O	2.18	0.43
1:A:174:PHE:CE2	2:B:165:THR:HG23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:188:GLU:O	2:H:189:LYS:HB2	2.19	0.43
2:K:35:TYR:HA	2:K:46:VAL:HG22	2.00	0.43
1:J:127:PRO:HD2	1:J:213:THR:HG21	2.00	0.43
1:A:34:THR:O	1:A:35:ALA:HB3	2.19	0.43
2:D:109:ARG:NH2	2:D:172:SER:O	2.52	0.43
2:D:111:VAL:O	2:D:111:VAL:CG1	2.66	0.43
2:B:46:VAL:O	2:B:47:ILE:HD13	2.18	0.43
2:B:176:LEU:HD12	2:B:177:SER:N	2.33	0.43
2:K:148:GLN:N	2:K:196:GLU:O	2.51	0.43
1:A:90:THR:CG2	1:A:91:PRO:HD2	2.49	0.42
1:G:76:ASP:O	1:G:80:ASN:N	2.52	0.42
1:A:14:PRO:HD2	1:J:180:SER:HA	2.01	0.42
1:G:4:LEU:HD21	1:G:22:CYS:SG	2.59	0.42
1:G:127:PRO:HD2	1:G:213:THR:HG21	2.00	0.42
2:H:135:CYS:HB2	2:H:149:TRP:CZ2	2.55	0.42
1:J:24:ILE:CD1	1:J:80:ASN:OD1	2.67	0.42
2:D:90:VAL:HG22	2:D:94:GLY:HA2	2.00	0.42
1:A:34:THR:HB	1:A:104:GLY:O	2.19	0.42
1:J:156:GLU:N	1:J:157:PRO:CD	2.82	0.42
2:K:111:VAL:O	2:K:111:VAL:CG1	2.65	0.42
2:D:141:TYR:O	2:D:174:TYR:CD2	2.72	0.42
2:H:27:LEU:H	2:H:68:THR:HA	1.85	0.42
1:C:17:THR:HG23	1:C:86:LEU:O	2.18	0.42
1:C:37:SER:OG	1:C:52:TRP:CD1	2.71	0.42
2:H:176:LEU:HD12	2:H:177:SER:H	1.84	0.42
2:K:11:SER:O	2:K:12:VAL:C	2.58	0.42
2:K:137:LEU:N	2:K:137:LEU:HD12	2.34	0.42
1:J:134:PRO:O	1:J:136:SER:N	2.49	0.42
1:C:35:ALA:HB3	1:C:102:GLY:N	2.35	0.42
1:C:11:LEU:HD21	1:C:122:ALA:O	2.20	0.42
2:H:147:VAL:HA	2:H:196:GLU:O	2.20	0.42
1:J:14:PRO:O	1:J:89:VAL:O	2.38	0.42
1:J:77:THR:C	1:J:79:LYS:O	2.58	0.42
1:C:18:LEU:HD11	1:C:117:VAL:HG11	2.02	0.41
1:G:156:GLU:N	1:G:157:PRO:CD	2.83	0.41
2:K:196:GLU:N	2:K:196:GLU:CD	2.74	0.41
1:J:178:LEU:HD13	1:J:184:TYR:CZ	2.54	0.41
2:K:85:TYR:O	2:K:102:GLY:HA2	2.20	0.41
2:H:90:VAL:HG22	2:H:94:GLY:HA2	2.02	0.41
2:K:170:LYS:C	2:K:172:SER:N	2.74	0.41
1:G:162:TRP:HB3	1:G:167:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:166:GLU:O	2:K:167:GLN:C	2.58	0.41
1:G:101:ARG:O	1:G:109:ASP:HA	2.21	0.41
1:J:54:TYR:CD1	1:J:60:PHE:HB2	2.55	0.41
2:H:12:VAL:HG23	2:H:105:LEU:HD13	2.03	0.41
2:H:141:TYR:CB	2:H:142:PRO:HD3	2.49	0.41
1:J:4:LEU:HD21	1:J:24:ILE:CG2	2.50	0.41
1:J:24:ILE:HD12	1:J:80:ASN:OD1	2.21	0.41
1:J:174:PHE:HA	2:K:165:THR:HG22	2.02	0.41
2:K:30:GLN:HG3	2:K:31:TYR:H	1.86	0.41
1:C:29:ILE:HD12	1:C:36:TRP:CD2	2.57	0.40
2:D:151:VAL:HG23	2:D:152:ASP:H	1.86	0.40
1:G:156:GLU:N	1:G:157:PRO:HD3	2.36	0.40
2:H:15:GLY:O	2:H:16:GLN:HG3	2.20	0.40
1:J:56:ARG:O	1:J:57:SER:C	2.59	0.40
1:C:71:VAL:HG12	1:C:86:LEU:HD13	2.02	0.40
2:H:164:VAL:CG2	2:H:176:LEU:HD13	2.50	0.40
1:J:20:LEU:HD12	1:J:84:LEU:HD23	2.02	0.40
1:C:158:VAL:HG12	1:C:208:HIS:ND1	2.36	0.40
2:H:151:VAL:CG2	2:H:154:ALA:HB3	2.51	0.40
1:C:127:PRO:HB3	1:C:150:VAL:HG12	2.03	0.40
2:D:105:LEU:HG	2:D:107:VAL:CG2	2.51	0.40
1:A:116:THR:HB	1:A:157:PRO:HG3	2.03	0.40
1:G:103:ASN:O	1:G:103:ASN:CG	2.59	0.40
2:H:164:VAL:HG12	2:H:165:THR:O	2.21	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 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	219/247 (89%)	202 (92%)	16 (7%)	1 (0%)	29 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	219/247 (89%)	198 (90%)	21 (10%)	0	100	100
1	G	215/247 (87%)	195 (91%)	19 (9%)	1 (0%)	29	64
1	J	207/247 (84%)	180 (87%)	26 (13%)	1 (0%)	29	64
2	B	212/215 (99%)	193 (91%)	17 (8%)	2 (1%)	17	52
2	D	212/215 (99%)	191 (90%)	20 (9%)	1 (0%)	29	64
2	H	212/215 (99%)	184 (87%)	23 (11%)	5 (2%)	6	27
2	K	193/215 (90%)	167 (86%)	22 (11%)	4 (2%)	7	30
3	E	5/14 (36%)	1 (20%)	4 (80%)	0	100	100
3	F	5/14 (36%)	4 (80%)	1 (20%)	0	100	100
All	All	1699/1876 (91%)	1515 (89%)	169 (10%)	15 (1%)	17	52

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
2	B	191	LYS
2	H	147	VAL
2	H	189	LYS
2	K	3	VAL
2	D	110	THR
2	B	125	GLN
2	H	26	ALA
2	K	107	VAL
2	K	147	VAL
2	H	170	LYS
1	J	37	SER
2	H	31	TYR
2	K	170	LYS
1	G	135	SER

### 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	191/212 (90%)	190 (100%)	1 (0%)	88	94
1	C	191/212 (90%)	187 (98%)	4 (2%)	53	79
1	G	189/212 (89%)	187 (99%)	2 (1%)	73	89
1	J	188/212 (89%)	184 (98%)	4 (2%)	53	79
2	B	183/184 (100%)	180 (98%)	3 (2%)	62	84
2	D	183/184 (100%)	180 (98%)	3 (2%)	62	84
2	H	183/184 (100%)	179 (98%)	4 (2%)	52	78
2	K	175/184 (95%)	173 (99%)	2 (1%)	73	89
3	E	7/14 (50%)	7 (100%)	0	100	100
3	F	7/14 (50%)	7 (100%)	0	100	100
All	All	1497/1612 (93%)	1474 (98%)	23 (2%)	65	85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	45	ARG
1	C	55	TYR
1	C	105	ASN
1	C	140	SER
2	D	2	TYR
2	D	31	TYR
2	D	166	GLU
1	A	1	GLN
2	B	60	ARG
2	B	87	CYS
2	B	191	LYS
1	G	146	LEU
1	G	181	SER
2	H	2	TYR
2	H	53	ARG
2	H	81	ASP
2	H	123	ASP
1	J	22	CYS
1	J	52	TRP
1	J	58	LYS
1	J	99	CYS
2	K	81	ASP
2	K	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

### 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](#)

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.

## 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, 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	221/247 (89%)	0.02	3 (1%) 75 56	34, 55, 101, 141	0
1	C	221/247 (89%)	-0.07	0 100 100	32, 44, 82, 113	0
1	G	219/247 (88%)	0.13	1 (0%) 91 81	33, 63, 108, 135	0
1	J	213/247 (86%)	0.30	11 (5%) 27 12	34, 73, 131, 153	0
2	B	214/215 (99%)	0.20	5 (2%) 60 39	41, 73, 114, 159	0
2	D	214/215 (99%)	0.10	0 100 100	34, 61, 85, 126	0
2	H	214/215 (99%)	0.12	1 (0%) 91 81	35, 80, 113, 138	0
2	K	203/215 (94%)	0.33	9 (4%) 34 17	40, 82, 136, 181	0
3	E	7/14 (50%)	1.60	2 (28%) 0 0	55, 67, 110, 122	0
3	F	7/14 (50%)	0.37	0 100 100	60, 61, 72, 72	0
All	All	1733/1876 (92%)	0.15	32 (1%) 68 47	32, 66, 117, 181	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	36	TRP	4.5
3	E	6	ASN	4.4
2	K	32	ALA	4.2
1	J	2	VAL	3.8
3	E	5	PRO	3.6
1	J	1	GLN	3.6
1	J	35	ALA	3.5
2	K	34	TRP	3.5
2	K	35	TYR	2.9
1	J	101	ARG	2.9
2	K	109	ARG	2.8
1	J	5	GLN	2.8
1	J	34	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	K	25	ASP	2.7
2	B	1	SER	2.6
2	H	27	LEU	2.6
1	A	45	ARG	2.6
1	A	108	MET	2.4
1	J	28	SER	2.5
1	J	75	PRO	2.4
2	B	195	CYS	2.4
1	A	107	GLY	2.4
2	K	88	GLN	2.4
1	J	25	SER	2.2
2	K	46	VAL	2.2
2	B	109	ARG	2.1
2	K	66	SER	2.1
1	G	3	GLN	2.0
1	J	74	ASN	2.0
2	B	186	ASP	2.0
2	B	156	GLN	2.0
2	K	110	THR	2.0

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.