



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:24 AM UTC

PDB ID : 5NB1 / pdb_00005nb1
Title : Crystal structures of homooligomers of collagen type IV. alpha4NC1
Authors : Casino, P.; Marina, A.
Deposited on : 2017-02-28
Resolution : 2.82 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

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
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

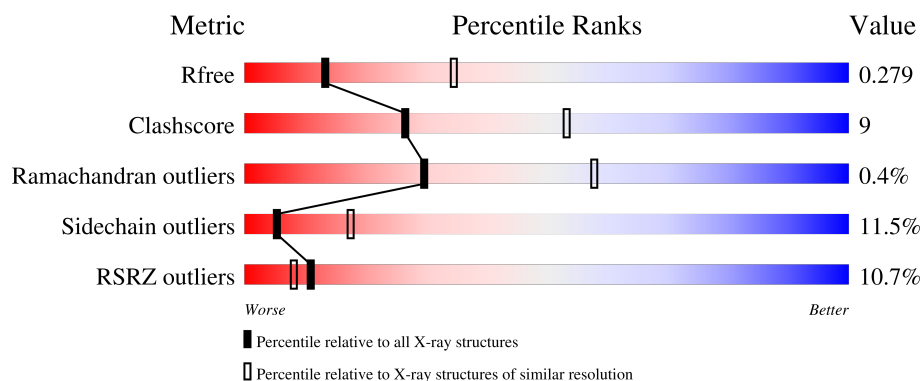
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	230	12% 66% 23% 9%
1	B	230	12% 67% 19% 10%
1	C	230	7% 66% 23% 10%
1	D	230	10% 63% 24% 10%
1	E	230	7% 68% 18% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	230	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9670 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-4(IV) chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	3	0
			1625	1030	282	296	17			
1	B	208	Total	C	N	O	S	0	1	0
			1607	1020	279	291	17			
1	C	208	Total	C	N	O	S	0	1	0
			1598	1015	276	292	15			
1	D	208	Total	C	N	O	S	0	1	0
			1592	1011	275	291	15			
1	E	206	Total	C	N	O	S	0	1	0
			1584	1008	274	285	17			
1	F	207	Total	C	N	O	S	0	2	0
			1597	1014	280	288	15			

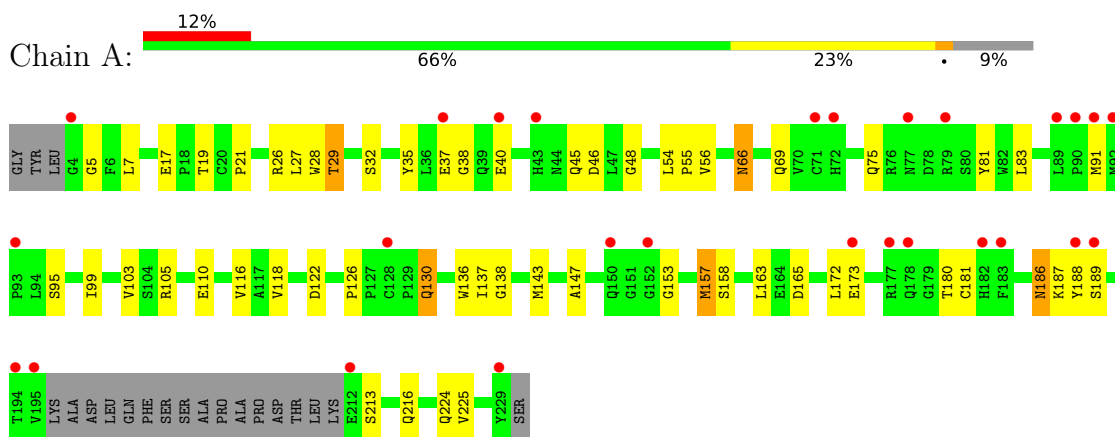
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	14	Total	O	0	0
			14	14		
2	C	11	Total	O	0	0
			11	11		
2	D	11	Total	O	0	0
			11	11		
2	E	3	Total	O	0	0
			3	3		
2	F	12	Total	O	0	0
			12	12		

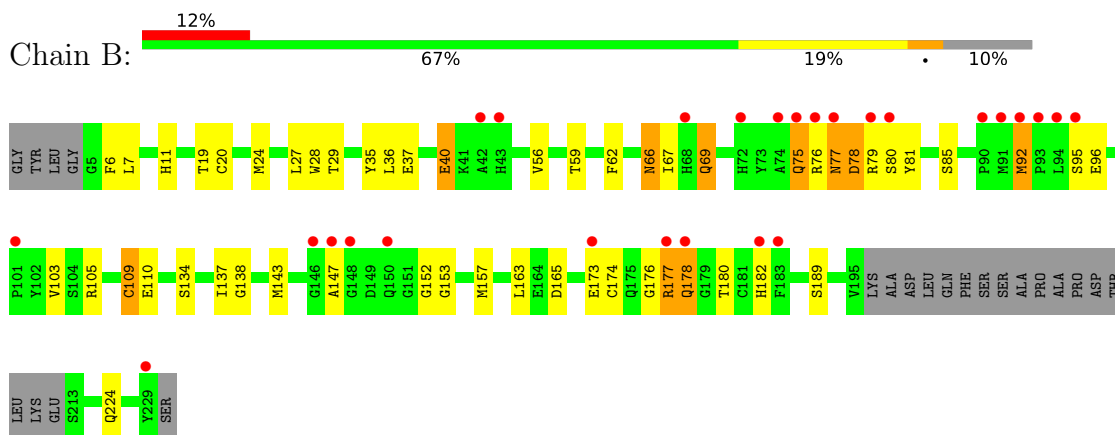
3 Residue-property plots [i](#)

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.

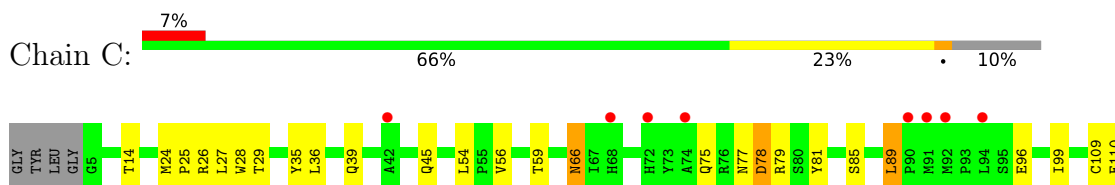
- Molecule 1: Collagen alpha-4(IV) chain

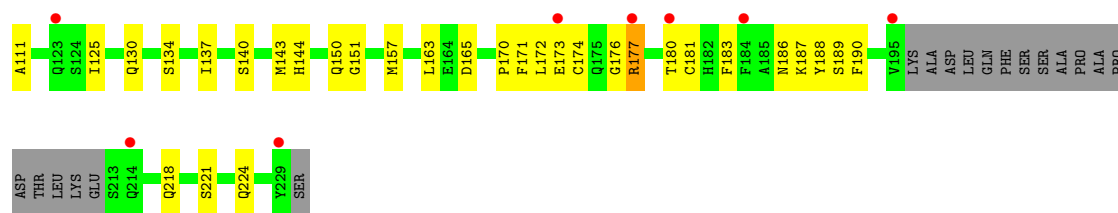


- Molecule 1: Collagen alpha-4(IV) chain

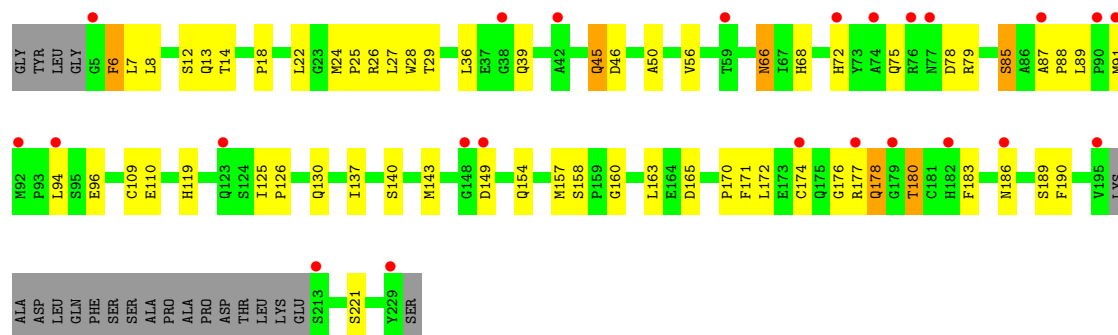


- Molecule 1: Collagen alpha-4(IV) chain

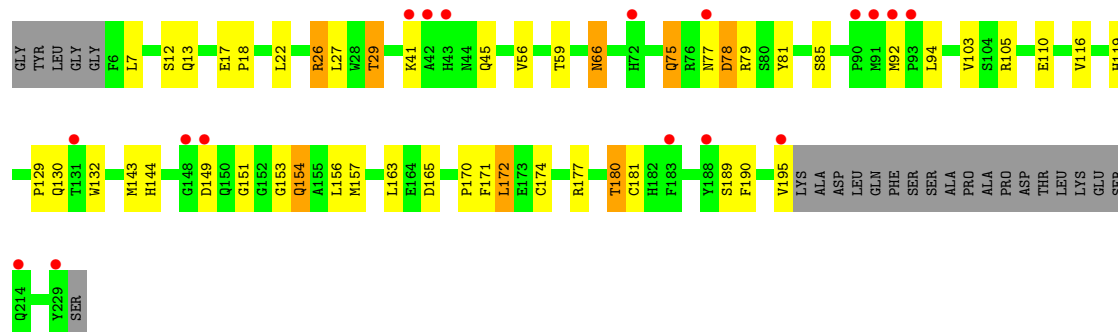




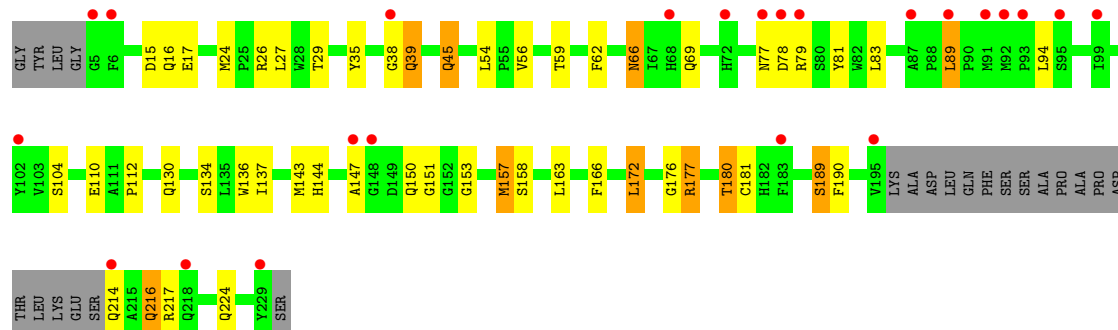
• Molecule 1: Collagen alpha-4(IV) chain



• Molecule 1: Collagen alpha-4(IV) chain



• Molecule 1: Collagen alpha-4(IV) chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	145.58Å 167.56Å 155.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.46 – 2.82 47.46 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.46-2.82) 99.7 (47.46-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.01 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.232 , 0.281 0.232 , 0.279	Depositor DCC
R_{free} test set	2376 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9670	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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 55.54 % 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 3.1155e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.84	0/1681	0.92	0/2289
1	B	0.83	1/1657 (0.1%)	1.04	8/2256 (0.4%)
1	C	0.86	0/1649	1.00	8/2249 (0.4%)
1	D	0.83	2/1642 (0.1%)	0.95	2/2240 (0.1%)
1	E	0.79	1/1634 (0.1%)	1.00	5/2228 (0.2%)
1	F	0.80	0/1650	0.98	9/2250 (0.4%)
All	All	0.83	4/9913 (0.0%)	0.98	32/13512 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	119	HIS	CG-CD2	5.10	1.41	1.35
1	D	126	PRO	C-O	-5.06	1.20	1.24
1	E	119	HIS	CG-CD2	5.05	1.41	1.35
1	B	11	HIS	CG-CD2	5.03	1.41	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	ASP	N-CA-C	10.05	123.29	111.02
1	E	77	ASN	N-CA-C	9.35	130.72	110.80
1	B	77	ASN	N-CA-C	9.29	123.72	108.96
1	E	78	ASP	N-CA-CB	-9.04	97.43	110.81
1	B	77	ASN	CB-CA-C	-8.56	95.92	110.22
1	E	130	GLN	N-CA-C	7.29	119.91	111.02
1	C	77	ASN	CB-CA-C	-6.62	97.25	110.42
1	F	89	LEU	CA-C-N	6.44	127.89	119.84
1	F	89	LEU	C-N-CA	6.44	127.89	119.84
1	C	77	ASN	N-CA-C	6.38	124.38	110.80
1	F	38	GLY	N-CA-C	6.24	127.96	113.18
1	F	130	GLN	N-CA-C	6.19	118.54	111.11
1	F	39	GLN	N-CA-C	6.07	119.39	110.59
1	B	78	ASP	N-CA-CB	-5.93	102.73	111.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	ASP	N-CA-C	5.86	123.28	110.80
1	B	78	ASP	N-CA-C	5.67	118.14	110.88
1	F	54	LEU	CA-C-N	5.66	125.34	119.05
1	F	54	LEU	C-N-CA	5.66	125.34	119.05
1	E	77	ASN	CB-CA-C	-5.61	99.27	110.42
1	C	78	ASP	N-CA-CB	-5.57	102.24	111.49
1	B	20	CYS	CA-C-N	5.43	125.43	120.21
1	B	20	CYS	C-N-CA	5.43	125.43	120.21
1	C	130	GLN	N-CA-C	5.31	120.13	111.37
1	D	130	GLN	N-CA-C	5.30	120.12	111.37
1	F	136	TRP	N-CA-C	5.29	116.88	108.79
1	C	111	ALA	CA-C-N	5.24	124.91	119.56
1	C	111	ALA	C-N-CA	5.24	124.91	119.56
1	B	75	GLN	N-CA-C	5.22	118.05	110.17
1	F	39	GLN	N-CA-CB	-5.20	102.51	110.42
1	B	76	ARG	N-CA-C	5.19	116.75	111.14
1	C	54	LEU	CA-C-N	5.12	124.73	119.05
1	C	54	LEU	C-N-CA	5.12	124.73	119.05

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	1625	0	1534	34	0
1	B	1607	0	1521	39	0
1	C	1598	0	1496	28	0
1	D	1592	0	1491	33	0
1	E	1584	0	1491	23	0
1	F	1597	0	1503	33	0
2	A	16	0	0	3	0
2	B	14	0	0	2	0
2	C	11	0	0	0	0
2	D	11	0	0	1	0
2	E	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	12	0	0	1	0
All	All	9670	0	9036	173	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 9.

All (173) 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:79:ARG:NH1	1:B:81:TYR:OH	2.04	0.90
1:A:137:ILE:CD1	1:A:224:GLN:HE21	1.89	0.86
1:B:153:GLY:HA3	1:D:28:TRP:CZ2	2.19	0.78
1:B:79:ARG:NH2	1:D:72:HIS:CE1	2.53	0.77
1:B:79:ARG:HH21	1:D:72:HIS:CE1	2.02	0.76
1:F:177:ARG:HH11	1:F:177:ARG:HG3	1.48	0.76
1:B:28:TRP:CE2	1:F:153:GLY:HA3	2.21	0.76
1:F:24:MET:HE2	1:F:112:PRO:HD2	1.69	0.74
1:A:137:ILE:HD11	1:A:224:GLN:HE21	1.55	0.72
1:B:78:ASP:HB2	1:B:176:GLY:HA3	1.70	0.72
1:E:154[A]:GLN:H	1:E:154[A]:GLN:HE21	1.37	0.71
1:B:59:THR:HG23	1:B:96:GLU:HG3	1.73	0.70
1:B:28:TRP:CZ2	1:F:153:GLY:HA3	2.27	0.69
1:D:68:HIS:O	1:D:72:HIS:HD2	1.74	0.69
1:B:153:GLY:HA3	1:D:28:TRP:CE2	2.28	0.68
1:C:78:ASP:HB2	1:C:176:GLY:HA3	1.75	0.67
1:A:153:GLY:HA3	1:C:28:TRP:CE2	2.31	0.67
1:A:95:SER:HB3	2:A:316:HOH:O	1.95	0.66
1:A:28:TRP:CE2	1:E:153:GLY:HA3	2.30	0.65
1:F:17:GLU:H	1:F:17:GLU:CD	2.03	0.65
1:C:81:TYR:CE2	1:C:173:GLU:HG3	2.31	0.65
1:D:186[B]:ASN:HD22	1:D:186[B]:ASN:H	1.43	0.65
1:F:177:ARG:HH11	1:F:177:ARG:CG	2.10	0.64
1:D:66:ASN:C	1:D:66:ASN:HD22	2.05	0.64
1:A:137:ILE:CD1	1:A:224:GLN:NE2	2.60	0.64
1:A:32:SER:HB3	1:A:83:LEU:HD12	1.81	0.63
1:B:37:GLU:OE1	1:B:79:ARG:HG3	2.00	0.62
1:D:46:ASP:OD2	1:D:158:SER:OG	2.09	0.61
1:B:75:GLN:O	1:B:177:ARG:NH1	2.32	0.60
1:C:78:ASP:O	1:C:176:GLY:N	2.34	0.60
1:C:134:SER:OG	1:C:224:GLN:NE2	2.35	0.60
1:A:137:ILE:HD11	1:A:224:GLN:NE2	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:LEU:HD23	1:D:50:ALA:HB2	1.85	0.59
1:E:26:ARG:HG2	1:E:26:ARG:HH11	1.69	0.58
1:E:66:ASN:C	1:E:66:ASN:HD22	2.12	0.58
1:D:78:ASP:O	1:D:176:GLY:N	2.36	0.58
1:C:187:LYS:HB3	1:C:188:TYR:CD2	2.39	0.58
1:B:134:SER:OG	1:B:224:GLN:NE2	2.37	0.58
1:D:170:PRO:HG2	1:D:171:PHE:CD2	2.40	0.56
1:D:6:PHE:CD1	1:D:6:PHE:N	2.73	0.56
1:B:77:ASN:OD1	1:B:77:ASN:O	2.24	0.56
1:A:122:ASP:HB2	2:A:303:HOH:O	2.05	0.56
1:A:66:ASN:C	1:A:66:ASN:HD22	2.15	0.55
1:B:78:ASP:HB2	1:B:176:GLY:CA	2.38	0.54
1:F:94:LEU:O	1:F:180:THR:HA	2.08	0.54
1:E:81:TYR:HA	1:E:172:LEU:O	2.07	0.54
1:A:46:ASP:OD2	1:A:158:SER:OG	2.25	0.54
1:F:39:GLN:HG3	1:F:45:GLN:HE22	1.72	0.54
1:A:21:PRO:HA	1:B:19:THR:OG1	2.08	0.54
1:F:137:ILE:HD13	1:F:224:GLN:HG3	1.89	0.54
1:E:26:ARG:HG2	1:E:26:ARG:NH1	2.23	0.53
1:E:143:MET:HG3	1:E:190:PHE:CE2	2.43	0.53
1:C:78:ASP:HB2	1:C:176:GLY:CA	2.38	0.53
1:C:66:ASN:C	1:C:66:ASN:HD22	2.16	0.53
1:F:81:TYR:HA	1:F:172:LEU:O	2.08	0.53
1:F:143:MET:HG3	1:F:190:PHE:CE2	2.44	0.53
1:F:214:GLN:HG3	1:F:217:ARG:HB3	1.92	0.52
1:E:79:ARG:HA	1:E:174:CYS:O	2.10	0.52
1:F:15:ASP:OD1	1:F:16[B]:GLN:NE2	2.42	0.52
1:F:157:MET:HE3	1:F:157:MET:HA	1.92	0.52
1:A:46:ASP:OD2	1:A:48:GLY:N	2.40	0.52
1:C:35:TYR:CG	1:C:143:MET:HE1	2.45	0.52
1:B:67:ILE:HD11	1:F:189:SER:HB3	1.90	0.52
1:C:89:LEU:HG	1:C:183:PHE:HB3	1.91	0.52
1:C:125:ILE:HG23	1:C:137:ILE:HG23	1.93	0.51
1:A:99:ILE:HG12	1:A:181:CYS:HB2	1.93	0.51
1:A:130[A]:GLN:HA	1:A:130[A]:GLN:OE1	2.10	0.51
1:D:143:MET:HG3	1:D:190:PHE:CD2	2.46	0.51
1:F:78:ASP:HB2	1:F:176:GLY:HA3	1.92	0.51
1:A:130[B]:GLN:HG2	2:A:314:HOH:O	2.10	0.51
1:C:39:GLN:HG3	1:C:45:GLN:HE22	1.74	0.50
1:B:134:SER:CB	1:B:224:GLN:HE21	2.23	0.50
1:B:134:SER:CB	1:B:224:GLN:NE2	2.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ASP:HB2	1:C:177:ARG:H	1.76	0.50
1:B:103:VAL:O	1:B:105[A]:ARG:NH2	2.45	0.50
1:D:14:THR:HA	1:D:85:SER:HB2	1.94	0.50
1:B:24:MET:CE	1:B:109:CYS:HB2	2.42	0.50
1:D:39:GLN:HG3	1:D:45:GLN:HE22	1.78	0.49
1:F:214:GLN:NE2	1:F:217:ARG:HD2	2.27	0.49
1:C:170:PRO:HG2	1:C:171:PHE:CD2	2.48	0.49
1:F:214:GLN:O	1:F:214:GLN:HG2	2.12	0.49
1:F:143:MET:HG3	1:F:190:PHE:CD2	2.48	0.49
1:B:134:SER:HB2	1:B:224:GLN:NE2	2.27	0.48
1:A:186:ASN:HD22	1:A:187:LYS:N	2.11	0.48
1:C:125:ILE:CG2	1:C:137:ILE:HG23	2.43	0.48
1:E:153:GLY:O	1:E:156:LEU:HB2	2.13	0.48
1:E:12:SER:HB3	1:E:18:PRO:HD3	1.95	0.48
1:C:143:MET:HG3	1:C:190:PHE:CE2	2.49	0.48
1:B:152:GLY:O	1:B:153:GLY:C	2.56	0.47
1:D:140:SER:HB2	1:D:221:SER:HB3	1.95	0.47
1:F:77:ASN:HA	1:F:79:ARG:HH11	1.79	0.47
1:C:99:ILE:HG12	1:C:181:CYS:HB2	1.97	0.47
1:A:81:TYR:CE2	1:A:173:GLU:HG3	2.50	0.47
1:E:59:THR:HG22	1:E:181:CYS:SG	2.55	0.47
1:B:6:PHE:N	1:B:6:PHE:CD1	2.83	0.46
1:A:17:GLU:HG2	1:A:29:THR:HG21	1.98	0.46
1:B:137:ILE:HG22	1:B:138:GLY:N	2.30	0.46
1:A:188:TYR:CZ	1:A:216:GLN:HG3	2.51	0.46
1:B:67:ILE:CD1	1:F:189:SER:HB3	2.46	0.46
1:E:170:PRO:HG2	1:E:171:PHE:CD2	2.50	0.46
1:B:80:SER:OG	1:B:174:CYS:HB2	2.16	0.46
1:D:79:ARG:HA	1:D:174:CYS:O	2.16	0.46
1:B:182:HIS:CE1	2:B:301:HOH:O	2.69	0.46
1:B:62:PHE:CE1	1:B:78:ASP:HA	2.51	0.45
1:C:14:THR:HA	1:C:85:SER:HB2	1.98	0.45
1:D:12:SER:HB3	1:D:18:PRO:HD3	1.97	0.45
1:D:91:MET:HA	1:D:183:PHE:CE1	2.51	0.45
1:A:137:ILE:HG22	1:A:138:GLY:N	2.31	0.45
1:B:147:ALA:HB3	1:D:36:LEU:HD11	1.99	0.45
1:D:94:LEU:O	1:D:180:THR:HG22	2.16	0.45
1:E:75:GLN:O	1:E:177:ARG:NH1	2.46	0.45
1:A:46:ASP:CG	1:A:158:SER:HG	2.24	0.45
1:A:28:TRP:CZ2	1:E:153:GLY:HA3	2.51	0.45
1:C:79:ARG:HA	1:C:174:CYS:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:PRO:HG2	1:E:132:TRP:CD2	2.52	0.44
1:A:153:GLY:HA3	1:C:28:TRP:CZ2	2.52	0.44
1:D:8:LEU:HA	2:D:306:HOH:O	2.16	0.44
1:F:35:TYR:CG	1:F:143:MET:HE1	2.52	0.44
1:F:62:PHE:CE1	1:F:78:ASP:HA	2.52	0.44
1:A:37:GLU:O	1:A:38:GLY:C	2.60	0.44
1:A:103:VAL:O	1:A:105[A]:ARG:NH2	2.50	0.44
1:B:95:SER:HB3	2:B:313:HOH:O	2.17	0.44
1:E:94:LEU:O	1:E:180:THR:HA	2.17	0.44
1:A:105[B]:ARG:HH11	1:E:195:VAL:HG13	1.83	0.44
1:C:143:MET:HG3	1:C:190:PHE:CD2	2.53	0.44
1:B:37:GLU:HB2	1:B:79:ARG:HB2	2.00	0.43
1:D:13:GLN:O	1:D:85:SER:HA	2.17	0.43
1:A:118:VAL:HG23	1:A:126:PRO:HG2	1.99	0.43
1:A:157:MET:HA	1:A:157:MET:HE3	2.00	0.43
1:F:59:THR:HG22	1:F:181:CYS:SG	2.58	0.43
1:D:94:LEU:O	1:D:180:THR:HA	2.17	0.43
1:E:13:GLN:O	1:E:85:SER:HA	2.18	0.43
1:D:143:MET:HG3	1:D:190:PHE:CE2	2.53	0.43
1:A:147:ALA:HB3	1:C:36:LEU:HD11	2.01	0.43
1:E:66:ASN:C	1:E:66:ASN:ND2	2.77	0.43
1:E:103:VAL:O	1:E:105:ARG:NH2	2.52	0.43
1:C:24:MET:HA	1:C:25:PRO:HD3	1.87	0.43
1:B:36:LEU:HD11	1:F:147:ALA:HB3	2.01	0.43
1:B:69:GLN:H	1:B:69:GLN:HG3	1.62	0.43
1:F:83:LEU:HB2	1:F:104:SER:HB3	2.01	0.42
1:B:176:GLY:C	1:B:178:GLN:H	2.27	0.42
1:A:54:LEU:HA	1:A:55:PRO:HD3	1.92	0.42
1:C:59:THR:HG23	1:C:96:GLU:HG3	2.00	0.42
1:C:140:SER:HB2	1:C:221:SER:HB3	2.02	0.42
1:D:176:GLY:C	1:D:178:GLN:H	2.28	0.42
1:F:144:HIS:CD2	1:F:151:GLY:HA2	2.54	0.42
1:B:40:GLU:H	1:B:40:GLU:CD	2.26	0.42
1:D:24:MET:HA	1:D:25:PRO:HD3	1.86	0.42
1:B:79:ARG:HD2	1:B:173:GLU:OE2	2.20	0.41
1:C:144:HIS:CD2	1:C:151:GLY:HA2	2.55	0.41
1:E:144:HIS:CD2	1:E:151:GLY:HA2	2.54	0.41
1:D:176:GLY:O	1:D:178:GLN:N	2.53	0.41
1:F:69:GLN:H	1:F:69:GLN:HG3	1.60	0.41
1:F:158:SER:HB3	2:F:301:HOH:O	2.21	0.41
1:E:81:TYR:CD1	1:E:81:TYR:N	2.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:SER:OG	1:F:224:GLN:NE2	2.45	0.41
1:D:158:SER:C	1:D:160:GLY:N	2.78	0.41
1:B:92:MET:H	1:B:92:MET:HG3	1.46	0.41
1:F:214:GLN:O	1:F:214:GLN:CG	2.68	0.41
1:C:137:ILE:HD13	1:C:224:GLN:HG3	2.03	0.40
1:C:78:ASP:CB	1:C:177:ARG:H	2.34	0.40
1:D:125:ILE:HG23	1:D:137:ILE:HG23	2.03	0.40
1:F:66:ASN:HD22	1:F:66:ASN:C	2.28	0.40
1:A:35:TYR:CG	1:A:143:MET:HE1	2.57	0.40
1:A:136:TRP:CZ2	1:A:225:VAL:HG21	2.57	0.40
1:E:17:GLU:HG2	1:E:29:THR:HG21	2.02	0.40
1:B:35:TYR:CG	1:B:143:MET:HE1	2.57	0.40
1:B:66:ASN:C	1:B:66:ASN:HD22	2.29	0.40
1:D:87:ALA:HA	1:D:88:PRO:HD3	1.94	0.40
1:F:166:PHE:CZ	1:F:216:GLN:HB3	2.56	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	209/230 (91%)	197 (94%)	11 (5%)	1 (0%)	24	53
1	B	205/230 (89%)	194 (95%)	10 (5%)	1 (0%)	24	53
1	C	205/230 (89%)	195 (95%)	9 (4%)	1 (0%)	24	53
1	D	205/230 (89%)	194 (95%)	9 (4%)	2 (1%)	12	36
1	E	203/230 (88%)	192 (95%)	11 (5%)	0	100	100
1	F	205/230 (89%)	191 (93%)	14 (7%)	0	100	100
All	All	1232/1380 (89%)	1163 (94%)	64 (5%)	5 (0%)	30	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	177	ARG
1	D	177	ARG
1	B	177	ARG
1	D	96	GLU
1	A	5	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	173/191 (91%)	149 (86%)	24 (14%)	3	11
1	B	171/191 (90%)	154 (90%)	17 (10%)	7	23
1	C	169/191 (88%)	151 (89%)	18 (11%)	6	20
1	D	168/191 (88%)	147 (88%)	21 (12%)	4	15
1	E	167/191 (87%)	145 (87%)	22 (13%)	4	13
1	F	168/191 (88%)	152 (90%)	16 (10%)	8	25
All	All	1016/1146 (89%)	898 (88%)	118 (12%)	5	17

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	19	THR
1	A	26	ARG
1	A	27	LEU
1	A	29	THR
1	A	40	GLU
1	A	45	GLN
1	A	56	VAL
1	A	66	ASN
1	A	69	GLN
1	A	75	GLN
1	A	91	MET
1	A	110	GLU
1	A	116	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	130[A]	GLN
1	A	130[B]	GLN
1	A	157	MET
1	A	163	LEU
1	A	165	ASP
1	A	172	LEU
1	A	180	THR
1	A	186	ASN
1	A	189	SER
1	A	213	SER
1	B	7	LEU
1	B	27	LEU
1	B	29	THR
1	B	40	GLU
1	B	56	VAL
1	B	66	ASN
1	B	69	GLN
1	B	85	SER
1	B	92	MET
1	B	109	CYS
1	B	110	GLU
1	B	157	MET
1	B	163	LEU
1	B	165	ASP
1	B	178	GLN
1	B	180	THR
1	B	189	SER
1	C	26	ARG
1	C	27	LEU
1	C	29	THR
1	C	56	VAL
1	C	66	ASN
1	C	75	GLN
1	C	89	LEU
1	C	109	CYS
1	C	110	GLU
1	C	150	GLN
1	C	157	MET
1	C	163	LEU
1	C	165	ASP
1	C	172	LEU
1	C	180	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	186	ASN
1	C	189	SER
1	C	218	GLN
1	D	6	PHE
1	D	22	LEU
1	D	26	ARG
1	D	27	LEU
1	D	29	THR
1	D	45	GLN
1	D	56	VAL
1	D	66	ASN
1	D	75	GLN
1	D	85	SER
1	D	89	LEU
1	D	109	CYS
1	D	110	GLU
1	D	154	GLN
1	D	157	MET
1	D	163	LEU
1	D	165	ASP
1	D	172	LEU
1	D	178	GLN
1	D	180	THR
1	D	189	SER
1	E	7	LEU
1	E	22	LEU
1	E	26	ARG
1	E	27	LEU
1	E	29	THR
1	E	41	LYS
1	E	45	GLN
1	E	56	VAL
1	E	66	ASN
1	E	75	GLN
1	E	78	ASP
1	E	92	MET
1	E	110	GLU
1	E	116	VAL
1	E	154[A]	GLN
1	E	154[B]	GLN
1	E	157	MET
1	E	163	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	165	ASP
1	E	172	LEU
1	E	180	THR
1	E	189	SER
1	F	26	ARG
1	F	27	LEU
1	F	29	THR
1	F	45	GLN
1	F	56	VAL
1	F	66	ASN
1	F	89	LEU
1	F	110	GLU
1	F	150	GLN
1	F	157	MET
1	F	163	LEU
1	F	172	LEU
1	F	177	ARG
1	F	180	THR
1	F	189	SER
1	F	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	66	ASN
1	A	114	GLN
1	A	186	ASN
1	A	224	GLN
1	B	16	GLN
1	B	39	GLN
1	B	114	GLN
1	B	154	GLN
1	B	224	GLN
1	C	16	GLN
1	C	66	ASN
1	C	77	ASN
1	C	144	HIS
1	C	224	GLN
1	D	43	HIS
1	D	66	ASN
1	D	72	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	77	ASN
1	D	123	GLN
1	D	150	GLN
1	E	66	ASN
1	E	114	GLN
1	E	123	GLN
1	E	144	HIS
1	F	43	HIS
1	F	66	ASN
1	F	123	GLN
1	F	182	HIS
1	F	214	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	210/230 (91%)	0.67	27 (12%) 7 5	22, 48, 101, 122	3 (1%)
1	B	208/230 (90%)	0.66	27 (12%) 7 5	22, 48, 92, 129	1 (0%)
1	C	208/230 (90%)	0.64	16 (7%) 19 14	26, 51, 93, 121	1 (0%)
1	D	208/230 (90%)	0.63	24 (11%) 9 7	23, 51, 92, 108	1 (0%)
1	E	206/230 (89%)	0.62	17 (8%) 17 12	27, 55, 97, 125	1 (0%)
1	F	207/230 (90%)	0.81	23 (11%) 10 7	28, 56, 97, 126	2 (0%)
All	All	1247/1380 (90%)	0.67	134 (10%) 11 8	22, 52, 95, 129	9 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	214	GLN	5.7
1	E	229	TYR	5.3
1	F	229	TYR	5.1
1	F	91	MET	4.7
1	C	229	TYR	4.6
1	F	68	HIS	4.6
1	E	42	ALA	4.3
1	B	229	TYR	4.3
1	B	91	MET	4.0
1	D	72	HIS	3.9
1	F	95	SER	3.9
1	F	38	GLY	3.9
1	B	146	GLY	3.8
1	D	229	TYR	3.7
1	B	76	ARG	3.7
1	F	72	HIS	3.6
1	F	214	GLN	3.6
1	A	183	PHE	3.6
1	F	77	ASN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	152	GLY	3.5
1	D	38	GLY	3.5
1	F	102	TYR	3.5
1	F	218	GLN	3.4
1	C	177	ARG	3.4
1	A	90	PRO	3.4
1	C	123	GLN	3.4
1	D	213	SER	3.3
1	E	91	MET	3.3
1	A	229	TYR	3.3
1	D	94	LEU	3.3
1	B	182	HIS	3.2
1	D	5	GLY	3.2
1	D	91	MET	3.2
1	A	189	SER	3.2
1	B	94	LEU	3.2
1	E	43	HIS	3.1
1	A	212	GLU	3.1
1	A	150	GLN	3.1
1	C	42	ALA	3.1
1	D	42	ALA	3.1
1	C	173	GLU	3.1
1	F	99	ILE	3.0
1	A	91	MET	3.0
1	E	183	PHE	3.0
1	B	150	GLN	3.0
1	C	180	THR	3.0
1	A	182	HIS	3.0
1	E	148	GLY	2.9
1	B	77	ASN	2.9
1	C	91	MET	2.9
1	E	92	MET	2.9
1	B	93	PRO	2.9
1	D	182	HIS	2.9
1	A	93	PRO	2.8
1	B	68	HIS	2.8
1	A	92	MET	2.8
1	F	5	GLY	2.8
1	C	68[A]	HIS	2.8
1	E	77	ASN	2.8
1	F	195	VAL	2.8
1	B	92	MET	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	214	GLN	2.7
1	D	123	GLN	2.7
1	A	37	GLU	2.7
1	F	87	ALA	2.7
1	C	72	HIS	2.7
1	F	183	PHE	2.7
1	A	194	THR	2.7
1	A	40	GLU	2.7
1	A	71	CYS	2.6
1	C	90	PRO	2.6
1	D	59	THR	2.6
1	C	94	LEU	2.6
1	F	147	ALA	2.6
1	A	173	GLU	2.6
1	B	74	ALA	2.6
1	B	43	HIS	2.5
1	A	89	LEU	2.5
1	F	79	ARG	2.5
1	C	195	VAL	2.4
1	A	79	ARG	2.4
1	D	92	MET	2.4
1	E	90	PRO	2.4
1	E	41	LYS	2.4
1	D	74	ALA	2.4
1	B	79	ARG	2.4
1	B	178	GLN	2.4
1	B	183	PHE	2.3
1	D	149	ASP	2.3
1	C	74	ALA	2.3
1	A	43	HIS	2.3
1	A	188	TYR	2.3
1	D	87	ALA	2.3
1	A	72	HIS	2.3
1	D	77	ASN	2.3
1	E	149	ASP	2.3
1	A	128	CYS	2.3
1	F	93	PRO	2.3
1	D	148	GLY	2.3
1	A	195	VAL	2.3
1	D	195	VAL	2.3
1	A	4	GLY	2.3
1	D	179	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	42	ALA	2.2
1	F	78	ASP	2.2
1	B	72	HIS	2.2
1	D	174	CYS	2.2
1	B	173	GLU	2.2
1	D	90	PRO	2.2
1	E	93	PRO	2.2
1	B	95	SER	2.2
1	F	148	GLY	2.2
1	C	184	PHE	2.2
1	A	77	ASN	2.2
1	B	75	GLN	2.2
1	B	177	ARG	2.2
1	E	131	THR	2.2
1	C	92	MET	2.2
1	B	90	PRO	2.2
1	E	195	VAL	2.2
1	B	147	ALA	2.2
1	D	76	ARG	2.1
1	D	186[A]	ASN	2.1
1	B	101	PRO	2.1
1	F	89	LEU	2.1
1	A	177	ARG	2.1
1	F	6	PHE	2.1
1	E	72	HIS	2.1
1	A	178	GLN	2.0
1	D	177	ARG	2.0
1	F	92	MET	2.0
1	B	80	SER	2.0
1	B	148	GLY	2.0
1	E	188	TYR	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 oligosaccharides 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.