Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:44 pm BST

PDB ID	:	5NB1
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 following versions of software and data (see references ①) were used in the production of this report:

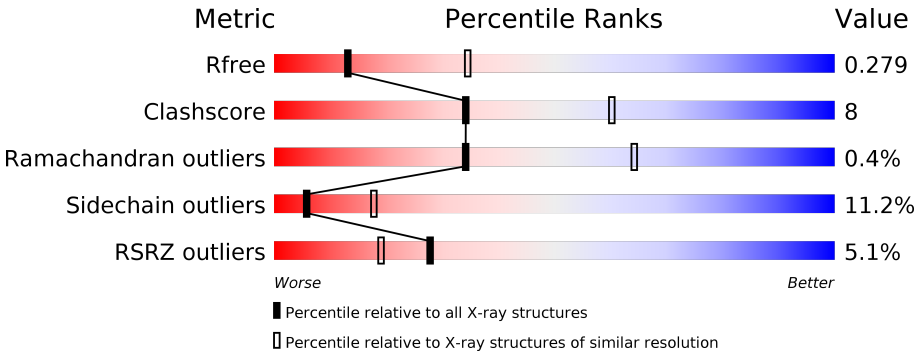
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.82 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (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 on 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 <=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	3% 67% 22% • 9%
1	B	230	5% 69% 20% • 10%
1	C	230	5% 67% 22% • 10%
1	D	230	2% 65% 23% • 10%
1	E	230	5% 68% 18% • 10%
1	F	230	7% 68% 19% • 10%

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.

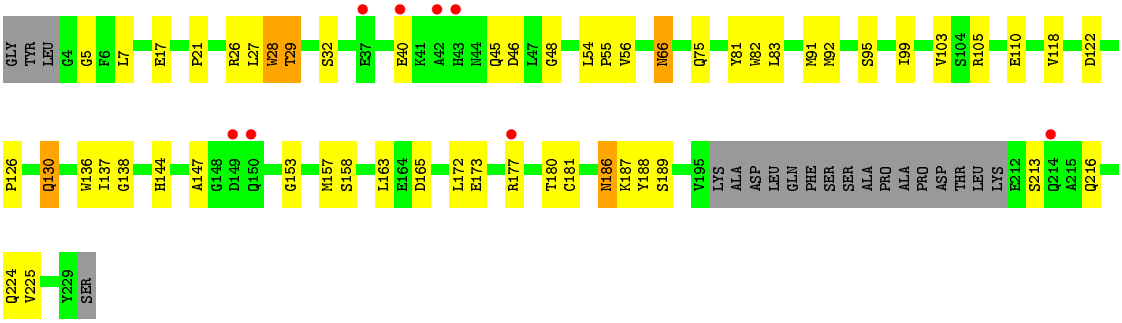
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	14	Total	O	0	0
			14	14		
2	C	11	Total	O	0	0
			11	11		
2	D	11	Total	O	0	0
			11	11		
2	E	3	Total	O	0	0
			3	3		
2	F	12	Total	O	0	0
			12	12		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

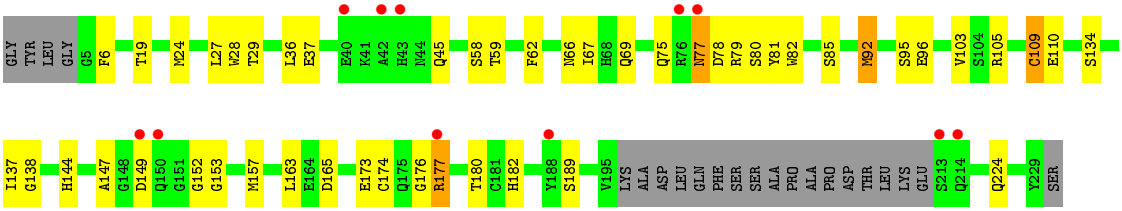
- Molecule 1: Collagen alpha-4(IV) chain

Chain A:



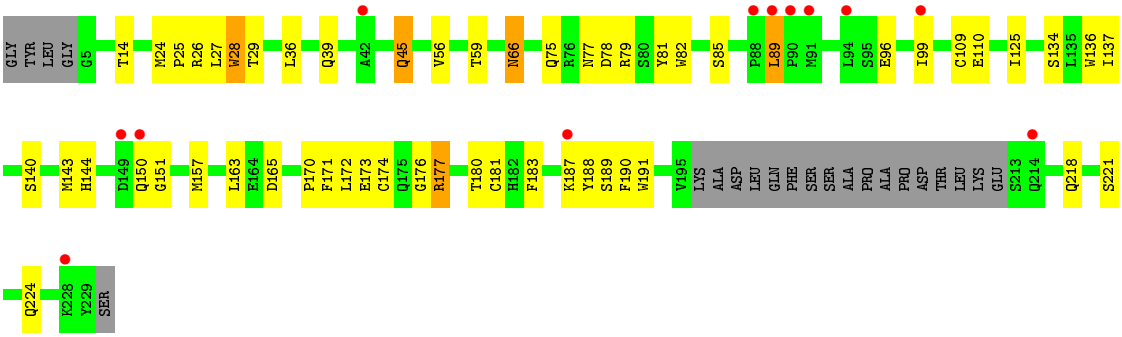
- Molecule 1: Collagen alpha-4(IV) chain

Chain B:



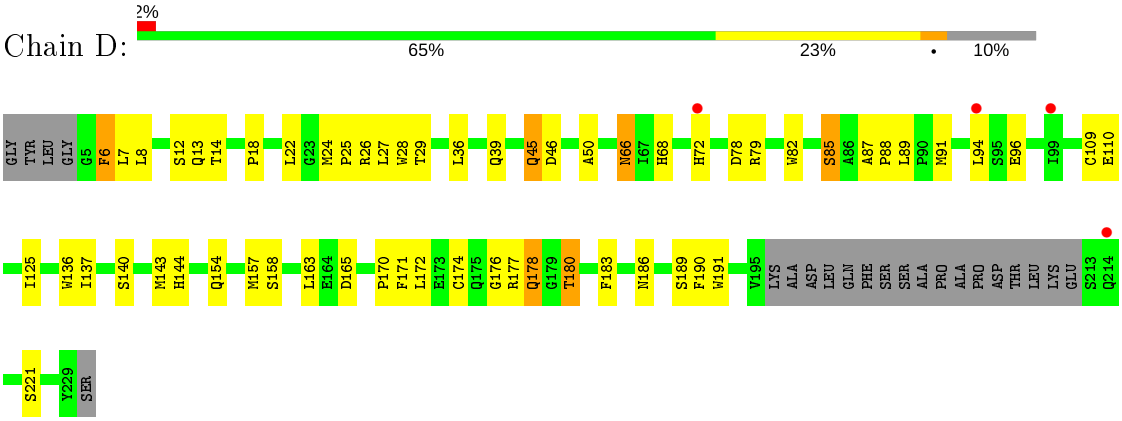
- Molecule 1: Collagen alpha-4(IV) chain

Chain C:



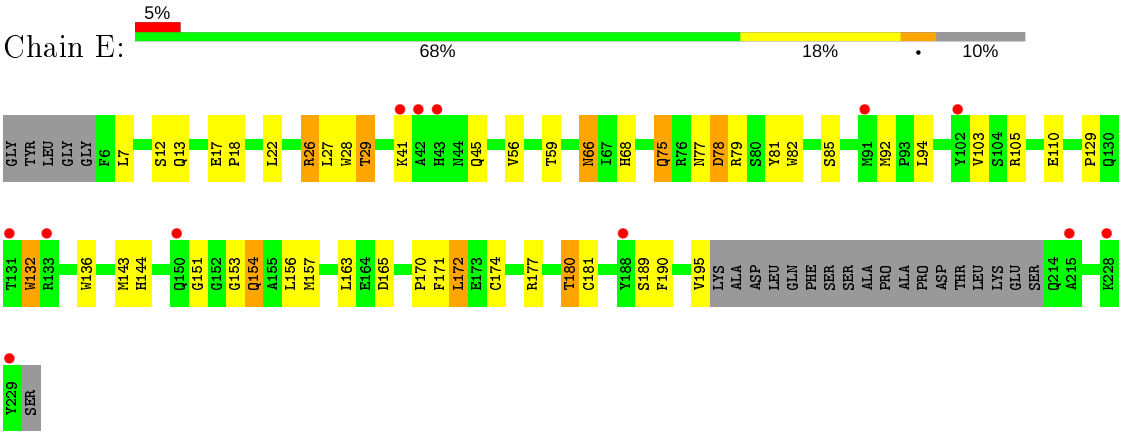
• Molecule 1: Collagen alpha-4(IV) chain

Chain D:



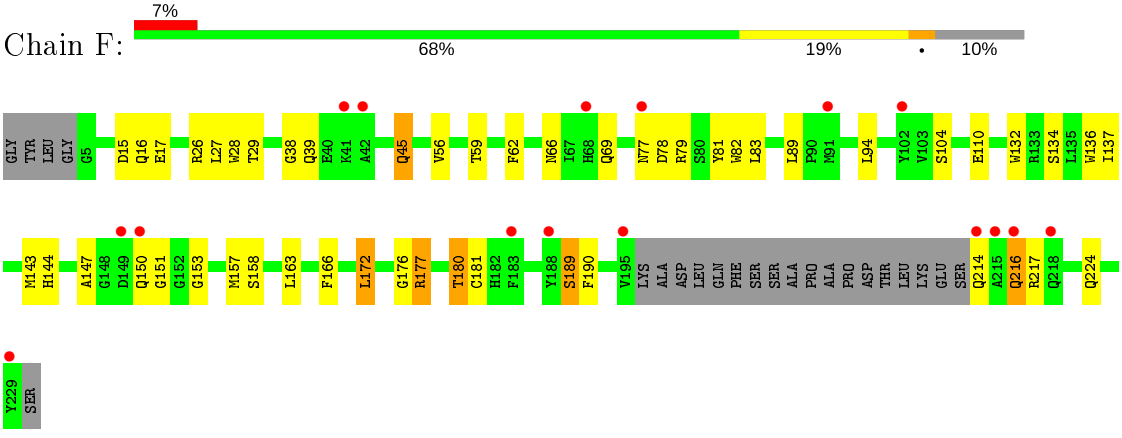
• Molecule 1: Collagen alpha-4(IV) chain

Chain E:



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

Chain F:



4 Data and refinement statistics (i)

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 46.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.46-2.82) 99.7 (46.86-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [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	2373 reflections (5.06%)	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)	0.34 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.68	2/1681 (0.1%)	0.67	0/2289
1	B	0.65	1/1657 (0.1%)	0.72	1/2256 (0.0%)
1	C	0.68	4/1649 (0.2%)	0.72	2/2249 (0.1%)
1	D	0.64	3/1642 (0.2%)	0.68	0/2240
1	E	0.62	4/1634 (0.2%)	0.72	3/2228 (0.1%)
1	F	0.63	4/1650 (0.2%)	0.69	1/2250 (0.0%)
All	All	0.65	18/9913 (0.2%)	0.70	7/13512 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	TRP	CD2-CE2	6.94	1.49	1.41
1	C	136	TRP	CD2-CE2	6.20	1.48	1.41
1	F	82	TRP	CD2-CE2	5.81	1.48	1.41
1	C	82	TRP	CD2-CE2	5.76	1.48	1.41
1	E	136	TRP	CD2-CE2	5.66	1.48	1.41
1	D	191	TRP	CD2-CE2	5.66	1.48	1.41
1	F	28	TRP	CD2-CE2	5.66	1.48	1.41
1	B	82	TRP	CD2-CE2	5.58	1.48	1.41
1	C	191	TRP	CD2-CE2	5.53	1.48	1.41
1	D	136	TRP	CD2-CE2	5.45	1.47	1.41
1	A	82	TRP	CD2-CE2	5.44	1.47	1.41
1	E	28	TRP	CD2-CE2	5.43	1.47	1.41
1	C	28	TRP	CD2-CE2	5.37	1.47	1.41
1	D	82	TRP	CD2-CE2	5.31	1.47	1.41
1	F	132	TRP	CD2-CE2	5.26	1.47	1.41
1	F	136	TRP	CD2-CE2	5.09	1.47	1.41
1	E	132	TRP	CD2-CE2	5.04	1.47	1.41
1	E	82	TRP	CD2-CE2	5.03	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	78	ASP	N-CA-CB	-7.32	97.43	110.60
1	E	77	ASN	N-CA-C	7.30	130.72	111.00
1	B	77	ASN	CB-CA-C	-7.24	95.92	110.40
1	C	77	ASN	CB-CA-C	-6.58	97.25	110.40
1	F	38	GLY	N-CA-C	5.94	127.96	113.10
1	E	77	ASN	CB-CA-C	-5.57	99.27	110.40
1	C	89	LEU	CA-CB-CG	5.56	128.08	115.30

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	1625	0	1534	30	0
1	B	1607	0	1521	35	0
1	C	1598	0	1496	27	0
1	D	1592	0	1491	31	0
1	E	1584	0	1491	22	0
1	F	1597	0	1503	29	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
2	F	12	0	0	1	0
All	All	9670	0	9036	157	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 8.

All (157) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:F:177:ARG:HH11	1.48	0.76
1:B:28:TRP:CE2	1:F:153:GLY:HA3	2.21	0.76
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:HE21	1:E:154[A]:GLN:H	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:C:81:TYR:CE2	1:C:173:GLU:HG3	2.31	0.65
1:D:186[B]:ASN:H	1:D:186[B]:ASN:HD22	1.43	0.65
1:F:177:ARG:HH11	1:F:177:ARG:CG	2.10	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:F:17:GLU:H	1:F:17:GLU:CD	2.03	0.60
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:D:66:ASN:C	1:D:66:ASN:HD22	2.05	0.59
1:A:137:ILE:HD11	1:A:224:GLN:NE2	2.17	0.59
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: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:N	1:D:6:PHE:CD1	2.73	0.56
1:B:77:ASN:O	1:B:77:ASN:OD1	2.24	0.56
1:A:122:ASP:HB2	2:A:303:HOH:O	2.05	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:66:ASN:C	1:E:66:ASN:HD22	2.12	0.53
1:E:143:MET:HG3	1:E:190:PHE:CE2	2.43	0.53
1:E:26:ARG:HG2	1:E:26:ARG:NH1	2.23	0.53
1:C:78:ASP:HB2	1:C:176:GLY:CA	2.38	0.53
1:F:143:MET:HG3	1:F:190:PHE:CE2	2.44	0.53
1:F:81:TYR:HA	1:F:172:LEU:O	2.08	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:A:46:ASP:OD2	1:A:48:GLY:N	2.40	0.52
1:C:89:LEU:HG	1:C:183:PHE:HB3	1.91	0.52
1:B:67:ILE:HD11	1:F:189:SER:HB3	1.90	0.52
1:C:125:ILE:HG23	1:C:137:ILE:HG23	1.93	0.51
1:A:130[A]:GLN:OE1	1:A:130[A]:GLN:HA	2.10	0.51
1:A:99:ILE:HG12	1:A:181:CYS:HB2	1.93	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:A:66:ASN:C	1:A:66:ASN:HD22	2.15	0.50
1:B:134:SER:CB	1:B:224:GLN:NE2	2.75	0.50
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:C:66:ASN:C	1:C:66:ASN:HD22	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CD1	1:B:6:PHE:N	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: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
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:62:PHE:CE1	1:F:78:ASP:HA	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:152:GLY:O	1:B:153:GLY:C	2.56	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: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:F:144:HIS:CD2	1:F:151:GLY:HA2	2.54	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:158:SER:HB3	2:F:301:HOH:O	2.21	0.41
1:F:69:GLN:HG3	1:F:69:GLN:H	1.60	0.41
1:E:81:TYR:N	1:E:81:TYR:CD1	2.87	0.41
1:F:134:SER:OG	1:F:224:GLN:NE2	2.45	0.41
1:B:92:MET:HG3	1:B:92:MET:H	1.46	0.41
1:F:214:GLN:CG	1:F:214:GLN:O	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: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:D:87:ALA:HA	1:D:88:PRO:HD3	1.94	0.40
1:A:46:ASP:CG	1:A:158:SER:HG	2.24	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%)	29	59
1	B	205/230 (89%)	194 (95%)	10 (5%)	1 (0%)	29	59
1	C	205/230 (89%)	195 (95%)	9 (4%)	1 (0%)	29	59
1	D	205/230 (89%)	194 (95%)	9 (4%)	2 (1%)	15	42
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%)	34	64

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 (i)

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	10
1	B	171/191 (90%)	155 (91%)	16 (9%)	8	25
1	C	169/191 (88%)	152 (90%)	17 (10%)	7	21
1	D	168/191 (88%)	148 (88%)	20 (12%)	5	15
1	E	167/191 (87%)	145 (87%)	22 (13%)	4	11
1	F	168/191 (88%)	152 (90%)	16 (10%)	8	24
All	All	1016/1146 (89%)	901 (89%)	115 (11%)	6	17

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
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	75	GLN
1	A	91	MET
1	A	92	MET
1	A	110	GLU
1	A	130[A]	GLN
1	A	130[B]	GLN
1	A	144	HIS
1	A	157	MET
1	A	163	LEU
1	A	165	ASP
1	A	172	LEU
1	A	177	ARG
1	A	180	THR
1	A	186	ASN
1	A	189	SER
1	A	213	SER
1	B	27	LEU
1	B	29	THR
1	B	45	GLN
1	B	58	SER
1	B	66	ASN
1	B	85	SER
1	B	92	MET
1	B	109	CYS
1	B	110	GLU
1	B	144	HIS
1	B	149	ASP
1	B	157	MET
1	B	163	LEU
1	B	165	ASP
1	B	180	THR
1	B	189	SER
1	C	26	ARG
1	C	27	LEU
1	C	29	THR

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Mol	Chain	Res	Type
1	C	45	GLN
1	C	56	VAL
1	C	66	ASN
1	C	75	GLN
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
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	66	ASN
1	D	85	SER
1	D	89	LEU
1	D	109	CYS
1	D	110	GLU
1	D	144	HIS
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

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Mol	Chain	Res	Type
1	E	66	ASN
1	E	68	HIS
1	E	75	GLN
1	E	78	ASP
1	E	92	MET
1	E	110	GLU
1	E	154[A]	GLN
1	E	154[B]	GLN
1	E	157	MET
1	E	163	LEU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	66	ASN
1	A	186	ASN
1	A	224	GLN
1	B	77	ASN
1	B	154	GLN
1	B	224	GLN
1	C	66	ASN

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Mol	Chain	Res	Type
1	C	224	GLN
1	D	43	HIS
1	D	66	ASN
1	D	72	HIS
1	D	123	GLN
1	D	150	GLN
1	E	123	GLN
1	E	186	ASN
1	F	123	GLN
1	F	182	HIS
1	F	214	GLN
1	F	224	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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%)	0.09	8 (3%) 40 30	27, 49, 101, 122	0
1	B	208/230 (90%)	0.11	11 (5%) 26 18	25, 48, 92, 129	0
1	C	208/230 (90%)	0.13	12 (5%) 23 15	26, 51, 93, 121	0
1	D	208/230 (90%)	0.13	4 (1%) 66 59	23, 51, 92, 108	0
1	E	206/230 (89%)	0.32	12 (5%) 23 15	28, 55, 97, 125	0
1	F	207/230 (90%)	0.35	16 (7%) 13 7	31, 56, 97, 126	0
All	All	1247/1380 (90%)	0.19	63 (5%) 28 19	23, 52, 95, 129	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	42	ALA	8.2
1	F	149	ASP	5.2
1	E	229	TYR	5.1
1	A	42	ALA	5.0
1	E	131	THR	4.9
1	B	42	ALA	4.8
1	F	214	GLN	4.6
1	A	214	GLN	4.4
1	C	91	MET	4.1
1	C	149	ASP	3.9
1	F	91	MET	3.7
1	A	43	HIS	3.7
1	B	213	SER	3.7
1	B	76	ARG	3.6
1	E	91	MET	3.5
1	E	188	TYR	3.5
1	A	40	GLU	3.5
1	B	188	TYR	3.5
1	B	43	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	42	ALA	3.3
1	D	94	LEU	3.3
1	F	102	TYR	3.2
1	E	215	ALA	3.2
1	C	214	GLN	3.1
1	A	150	GLN	2.9
1	C	42	ALA	2.9
1	C	90	PRO	2.9
1	F	183	PHE	2.8
1	D	72	HIS	2.8
1	B	149	ASP	2.8
1	F	41	LYS	2.8
1	C	89	LEU	2.7
1	E	43	HIS	2.7
1	B	150	GLN	2.7
1	D	214	GLN	2.6
1	F	215	ALA	2.6
1	D	99	ILE	2.6
1	B	214	GLN	2.6
1	E	41	LYS	2.6
1	F	188	TYR	2.5
1	E	133	ARG	2.5
1	C	94	LEU	2.5
1	A	177	ARG	2.5
1	F	216	GLN	2.5
1	E	228	LYS	2.4
1	F	229	TYR	2.4
1	A	37	GLU	2.3
1	C	88	PRO	2.3
1	F	68	HIS	2.3
1	C	187	LYS	2.3
1	F	77	ASN	2.2
1	F	150	GLN	2.2
1	B	77	ASN	2.2
1	A	149	ASP	2.2
1	B	177	ARG	2.2
1	F	218	GLN	2.2
1	B	40	GLU	2.2
1	F	195	VAL	2.2
1	E	102	TYR	2.1
1	C	228	LYS	2.1
1	E	150	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	150	GLN	2.0
1	C	99	ILE	2.0

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.