Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:01 AM GMT

PDB ID	:	2F9Z
Title	:	Complex between the chemotaxis deamidase CheD and the chemotaxis phosphatase CheC from Thermotoga maritima
Authors	:	Chao, X.; Park, S.Y; Bilwes, A.M.; Crane, B.R.
Deposited on	:	2005-12-06
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

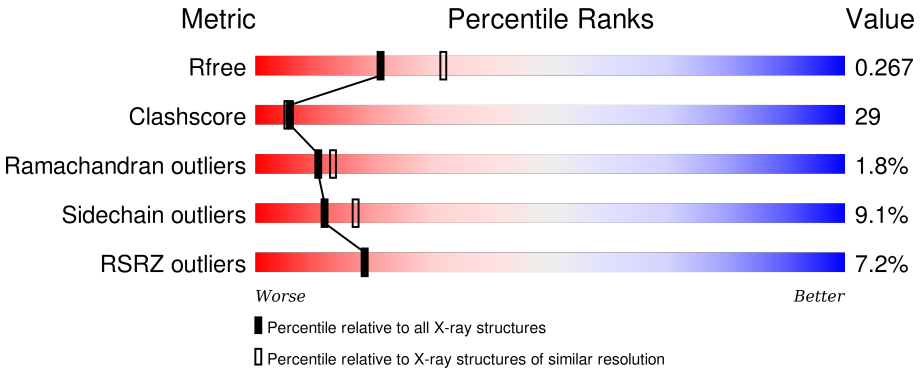
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	205	8% 47% 41% 6% 6%
1	B	205	12% 43% 45% 7%
2	C	159	3% 50% 44%
2	D	159	3% 50% 43%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5552 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 chemotaxis protein CheC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1452	939	222	281	10			
1	B	190	Total	C	N	O	S	0	0	0
			1433	930	224	268	11			

- Molecule 2 is a protein called PROTEIN (chemotaxis methylation protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	154	Total	C	N	O	S	0	0	0
			1140	719	201	210	10			
2	D	154	Total	C	N	O	S	0	0	0
			1135	715	202	209	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ALA	-	CLONING ARTIFACT	UNP Q9X005
C	0	HIS	-	CLONING ARTIFACT	UNP Q9X005
D	-1	ALA	-	CLONING ARTIFACT	UNP Q9X005
D	0	HIS	-	CLONING ARTIFACT	UNP Q9X005

- Molecule 3 is water.

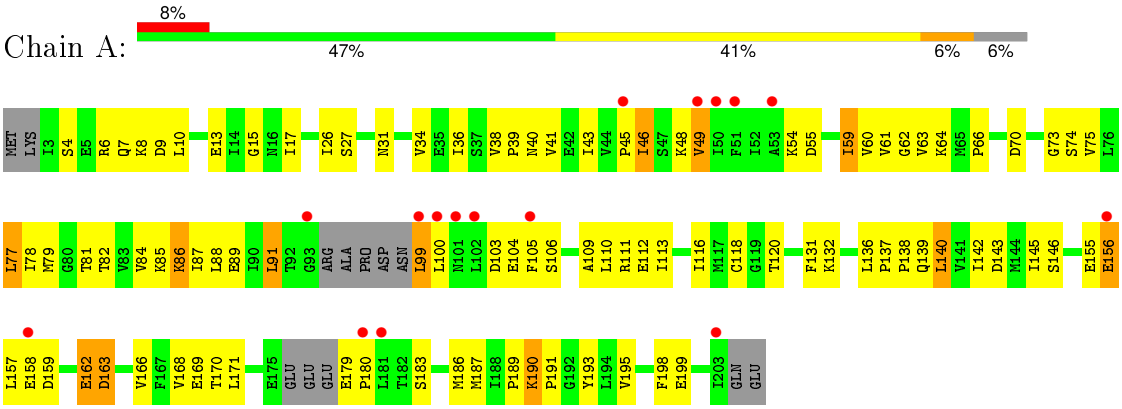
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total	O	0	0
			111	111		
3	B	100	Total	O	0	0
			100	100		
3	C	94	Total	O	0	0
			94	94		
3	D	87	Total	O	0	0
			87	87		

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 errors 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.

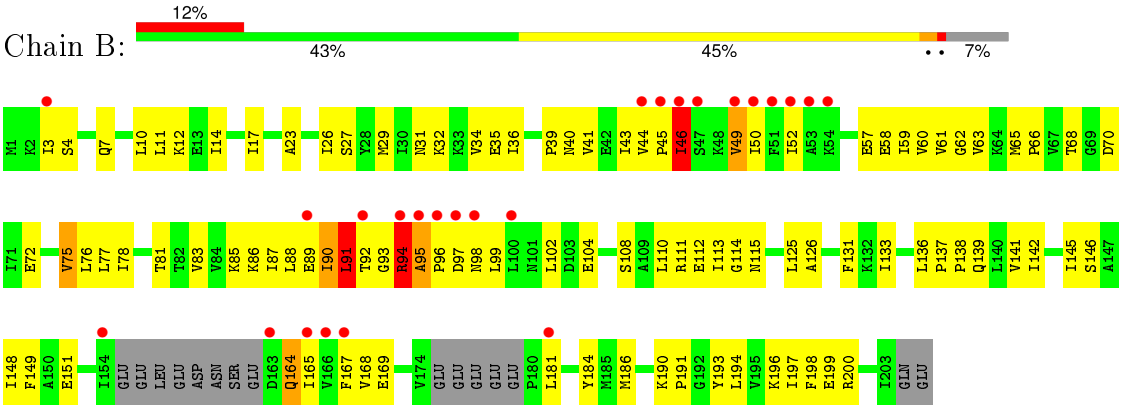
- Molecule 1: chemotaxis protein CheC

Chain A:



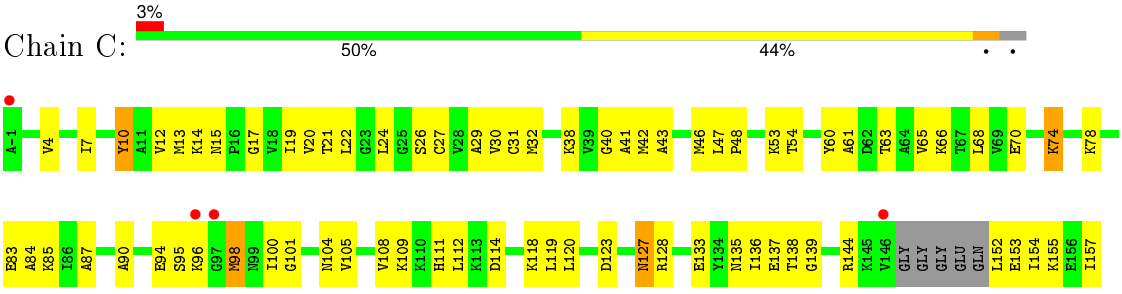
- Molecule 1: chemotaxis protein CheC

Chain B:



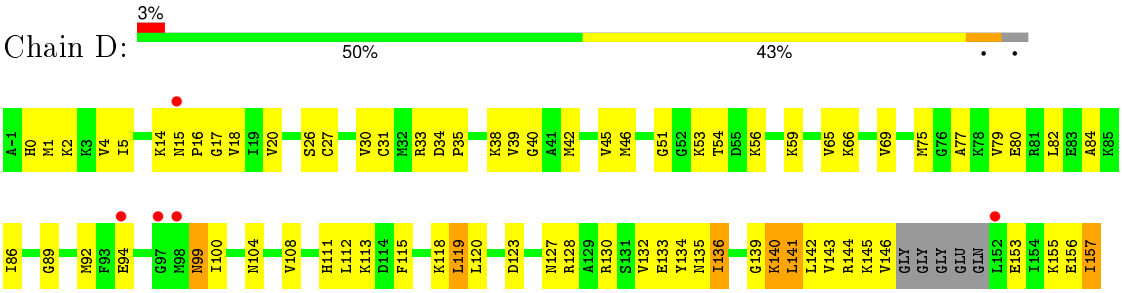
- Molecule 2: PROTEIN (chemotaxis methylation protein)

Chain C:



- Molecule 2: PROTEIN (chemotaxis methylation protein)

Chain D:


3%
50%
43%
A-1 H0 M1 K2 K3 V4 I5 K14 N15 P16 G17 V18 I19 V20 S26 C27 V30 C31 M32 R33 D34 P35 K38 V39 G40 A41 M42 V45 M46 G51 G52 K53 T54 D55 K56 K59 V65 K66 V69 M75 G76 A77 K78 V79 E80 R81 L82 E83 A84 K85
I86 G89 M92 F93 E94 G97 M98 N99 I100 N104 V108 H111 L112 K113 D114 F115 K118 L119 L120 D123 N127 R128 A129 R130 S131 V132 E133 Y134 N135 I136 G139 K140 L141 L142 V143 R144 K145 V146 GLY GLY GLY GLU GLN L152 E153 I154 K155 E156 I157

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	66.08Å 66.08Å 161.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.40 28.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.4 (30.00-2.40) 53.0 (28.61-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.275 0.211 , 0.267	Depositor DCC
R_{free} test set	1630 reflections (9.98%)	DCC
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 33.5	EDS
Estimated twinning fraction	0.186 for -h,-k,l 0.319 for h,-h-k,-l 0.217 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Outliers	0 of 16378 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5552	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.36	0/1468	0.65	0/1987
1	B	0.42	0/1450	0.67	1/1961 (0.1%)
2	C	0.42	1/1149 (0.1%)	0.68	1/1531 (0.1%)
2	D	0.38	0/1145	0.69	1/1527 (0.1%)
All	All	0.39	1/5212 (0.0%)	0.67	3/7006 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	157	ILE	C-OXT	-5.57	1.12	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	114	ASP	CB-CA-C	-6.43	97.54	110.40
1	B	164	GLN	N-CA-C	-6.12	94.48	111.00
2	D	17	GLY	N-CA-C	5.54	126.95	113.10

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	1452	0	1504	90	0
1	B	1433	0	1518	97	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1140	0	1220	65	0
2	D	1135	0	1202	59	0
3	A	111	0	0	10	0
3	B	100	0	0	18	0
3	C	94	0	0	6	0
3	D	87	0	0	6	0
All	All	5552	0	5444	305	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 29.

All (305) 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:A:45:PRO:HB3	1:A:163:ASP:HB3	1.33	1.11
1:A:190:LYS:HB3	1:A:191:PRO:HD2	1.41	1.00
1:A:66:PRO:HG2	1:A:136:LEU:HB2	1.49	0.94
2:D:39:VAL:HG21	2:D:75:MET:HG2	1.51	0.91
2:C:7:ILE:H	2:C:7:ILE:HD12	1.36	0.90
2:C:13:MET:HG2	2:C:17:GLY:HA3	1.53	0.89
1:A:59:ILE:H	1:A:59:ILE:HD13	1.36	0.89
1:B:49:VAL:HG21	1:B:165:ILE:HD11	1.54	0.88
1:A:158:GLU:HG2	1:A:159:ASP:H	1.39	0.85
2:D:1:MET:SD	2:D:16:PRO:HB2	2.17	0.84
1:B:26:ILE:HD12	1:B:36:ILE:HD11	1.59	0.83
2:C:135:ASN:HD21	2:C:137:GLU:HB3	1.44	0.82
1:B:165:ILE:HD12	1:B:186:MET:SD	2.19	0.81
2:D:42:MET:HG2	3:D:1237:HOH:O	1.82	0.80
1:B:77:LEU:HD23	1:B:114:GLY:HA2	1.63	0.80
2:C:127:ASN:HD22	2:C:127:ASN:H	1.29	0.79
1:B:78:ILE:HB	1:B:184:TYR:HB2	1.65	0.78
1:B:63:VAL:HG11	1:B:114:GLY:HA3	1.68	0.75
1:B:41:VAL:HG12	1:B:168:VAL:HG22	1.69	0.75
1:A:13:GLU:O	1:A:17:ILE:HG12	1.87	0.75
2:D:99:ASN:H	2:D:99:ASN:ND2	1.82	0.75
1:B:190:LYS:HB3	1:B:191:PRO:HD2	1.69	0.74
1:A:171:LEU:HD11	1:A:180:PRO:HB2	1.67	0.74
1:B:12:LYS:HD3	1:B:40:ASN:HA	1.70	0.73
1:B:46:ILE:H	1:B:46:ILE:HD13	1.53	0.73
2:D:99:ASN:HD22	2:D:99:ASN:N	1.86	0.72
1:A:89:GLU:HB3	3:A:1187:HOH:O	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:ALA:HB1	3:C:1067:HOH:O	1.92	0.70
1:B:133:ILE:HG13	3:B:1357:HOH:O	1.92	0.70
2:D:86:ILE:HG23	2:D:119:LEU:HD21	1.72	0.70
1:B:34:VAL:HB	3:B:1104:HOH:O	1.91	0.70
2:D:14:LYS:C	2:D:16:PRO:HD2	2.12	0.70
1:A:190:LYS:HB3	1:A:191:PRO:CD	2.20	0.69
1:B:77:LEU:CD2	1:B:114:GLY:HA2	2.22	0.69
1:B:99:LEU:HB3	1:B:142:ILE:HD13	1.74	0.69
1:B:167:PHE:CD1	1:B:186:MET:HB3	2.27	0.69
1:A:60:VAL:HG21	1:A:78:ILE:HG23	1.75	0.69
1:A:45:PRO:CB	1:A:163:ASP:HB3	2.18	0.69
1:A:41:VAL:HG22	1:A:168:VAL:HG13	1.75	0.68
1:B:151:GLU:HG3	2:D:92:MET:SD	2.34	0.68
2:D:99:ASN:HD22	2:D:99:ASN:H	1.40	0.68
2:C:135:ASN:HD22	2:C:138:THR:H	1.40	0.68
1:A:136:LEU:HB3	1:A:137:PRO:HD2	1.76	0.68
1:B:44:VAL:HG23	3:B:1151:HOH:O	1.93	0.68
2:C:10:TYR:HD2	2:C:68:LEU:HD12	1.60	0.67
1:B:81:THR:HG22	1:B:85:LYS:HE2	1.75	0.67
1:A:74:SER:HB3	3:A:1365:HOH:O	1.94	0.67
2:C:127:ASN:N	2:C:127:ASN:HD22	1.92	0.67
1:B:190:LYS:HB2	1:B:193:TYR:CD2	2.31	0.66
1:A:64:LYS:HE2	3:A:1365:HOH:O	1.96	0.65
2:D:18:VAL:HG11	2:D:133:GLU:HB3	1.79	0.65
1:A:109:ALA:O	1:A:113:ILE:HG13	1.96	0.65
2:D:27:CYS:HA	3:D:1165:HOH:O	1.95	0.65
1:B:89:GLU:O	1:B:91:LEU:N	2.30	0.65
2:C:19:ILE:HG13	3:C:1057:HOH:O	1.97	0.65
1:A:88:LEU:HD21	1:A:106:SER:OG	1.97	0.64
2:C:24:LEU:HD11	2:C:29:ALA:HB2	1.78	0.64
1:B:148:ILE:HB	3:B:1253:HOH:O	1.98	0.64
2:D:15:ASN:N	2:D:16:PRO:HD2	2.13	0.64
1:A:39:PRO:HD3	3:A:1220:HOH:O	1.97	0.63
1:A:45:PRO:HA	1:A:163:ASP:O	1.98	0.63
2:D:31:CYS:SG	2:D:42:MET:HG3	2.40	0.62
1:B:3:ILE:HA	3:B:1116:HOH:O	1.99	0.62
1:B:102:LEU:HD13	3:B:1236:HOH:O	2.00	0.62
2:C:15:ASN:HB2	2:C:38:LYS:HB3	1.80	0.62
1:B:89:GLU:HG3	1:B:94:ARG:HA	1.82	0.61
2:D:141:LEU:HD12	2:D:157:ILE:HD11	1.82	0.61
1:B:141:VAL:HG13	1:B:148:ILE:HD13	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:SER:O	1:A:110:LEU:HB2	2.01	0.61
1:A:45:PRO:HG2	1:A:48:LYS:CB	2.31	0.61
1:B:34:VAL:HG22	1:B:35:GLU:H	1.66	0.61
1:B:193:TYR:HA	1:B:196:LYS:HB2	1.83	0.61
1:B:86:LYS:HG3	1:B:90:ILE:HD13	1.82	0.60
1:B:60:VAL:O	1:B:142:ILE:HA	2.01	0.60
1:A:190:LYS:CB	1:A:191:PRO:HD2	2.24	0.60
1:B:34:VAL:HG22	1:B:35:GLU:N	2.17	0.60
1:B:95:ALA:N	1:B:96:PRO:CD	2.65	0.60
1:A:59:ILE:N	1:A:59:ILE:HD13	2.11	0.60
1:B:29:MET:HG2	3:B:1304:HOH:O	2.02	0.60
1:A:82:THR:O	1:A:86:LYS:HG2	2.02	0.59
2:D:84:ALA:H	2:D:120:LEU:HD13	1.67	0.59
2:D:65:VAL:O	2:D:69:VAL:HG13	2.03	0.59
1:B:39:PRO:HG2	1:B:169:GLU:HG3	1.85	0.59
1:A:189:PRO:HB2	1:A:193:TYR:HB2	1.84	0.58
2:C:22:LEU:HD23	3:C:1356:HOH:O	2.03	0.58
2:C:7:ILE:H	2:C:7:ILE:CD1	2.12	0.58
1:A:99:LEU:HG	1:A:142:ILE:HG21	1.85	0.58
1:B:164:GLN:O	1:B:194:LEU:HD22	2.03	0.58
1:A:156:GLU:HG3	1:A:157:LEU:H	1.67	0.58
1:A:41:VAL:HG13	1:A:168:VAL:HG22	1.85	0.58
1:B:44:VAL:HB	1:B:45:PRO:HD2	1.83	0.58
2:D:77:ALA:HB1	2:D:82:LEU:HD11	1.85	0.58
2:D:133:GLU:HB2	2:D:142:LEU:HB3	1.86	0.58
2:C:32:MET:HA	2:C:83:GLU:O	2.03	0.58
1:B:11:LEU:HB2	1:B:41:VAL:HG21	1.85	0.58
2:C:128:ARG:HH12	2:C:152:LEU:HD13	1.69	0.58
2:C:19:ILE:HG21	2:C:42:MET:HB3	1.85	0.57
1:B:190:LYS:HB2	1:B:193:TYR:HD2	1.68	0.57
1:B:131:PHE:CZ	1:B:200:ARG:HG3	2.39	0.57
2:C:109:LYS:HE3	2:C:119:LEU:HD12	1.86	0.57
1:B:27:SER:HB2	1:B:34:VAL:HG12	1.86	0.57
1:A:63:VAL:CG1	1:A:138:PRO:HB2	2.34	0.57
1:A:64:LYS:HD3	1:A:139:GLN:NE2	2.19	0.57
2:D:30:VAL:HG22	2:D:108:VAL:HG21	1.86	0.57
1:A:156:GLU:HG3	1:A:157:LEU:N	2.20	0.57
1:A:59:ILE:H	1:A:59:ILE:CD1	2.07	0.56
1:B:89:GLU:C	1:B:91:LEU:H	2.08	0.56
2:D:145:LYS:HG2	3:D:1031:HOH:O	2.05	0.56
1:B:26:ILE:HG22	3:B:1104:HOH:O	2.03	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ASP:O	1:A:13:GLU:HG3	2.05	0.56
1:B:95:ALA:N	1:B:96:PRO:HD2	2.20	0.56
1:B:50:ILE:HA	3:B:1303:HOH:O	2.05	0.56
1:A:43:ILE:HG12	1:A:198:PHE:HZ	1.70	0.56
2:D:145:LYS:O	2:D:153:GLU:HG3	2.06	0.56
1:B:96:PRO:HA	3:B:1236:HOH:O	2.06	0.55
2:D:123:ASP:OD2	2:D:143:VAL:HG11	2.05	0.55
1:B:39:PRO:HD2	1:B:169:GLU:O	2.06	0.55
1:A:60:VAL:HG23	1:A:79:MET:O	2.06	0.55
1:B:60:VAL:HG21	3:B:1253:HOH:O	2.07	0.55
2:D:135:ASN:O	2:D:139:GLY:N	2.40	0.55
1:A:171:LEU:N	3:A:1220:HOH:O	2.40	0.55
1:B:91:LEU:HD23	1:B:92:THR:HG23	1.89	0.54
1:A:84:VAL:HG13	1:A:110:LEU:HD11	1.89	0.54
1:B:145:ILE:HA	3:B:1253:HOH:O	2.07	0.54
2:D:4:VAL:HA	2:D:20:VAL:O	2.07	0.54
1:A:70:ASP:HB3	1:A:131:PHE:CD2	2.43	0.54
1:A:170:THR:OG1	1:A:183:SER:HB2	2.08	0.54
1:A:55:ASP:O	1:A:145:ILE:HG21	2.07	0.53
2:C:61:ALA:O	2:C:65:VAL:HG12	2.07	0.53
1:A:46:ILE:H	1:A:46:ILE:HD13	1.74	0.53
1:A:70:ASP:HB3	1:A:131:PHE:HD2	1.73	0.53
1:A:159:ASP:HA	2:C:46:MET:CE	2.39	0.53
1:A:112:GLU:O	1:A:116:ILE:HG13	2.09	0.53
2:D:111:HIS:O	2:D:115:PHE:HD1	1.91	0.53
2:D:1:MET:SD	2:D:16:PRO:CB	2.93	0.52
1:A:158:GLU:HG2	1:A:159:ASP:N	2.16	0.52
1:A:171:LEU:HB2	3:A:1220:HOH:O	2.09	0.52
1:A:4:SER:O	1:A:8:LYS:HG3	2.09	0.52
1:B:89:GLU:C	1:B:91:LEU:N	2.63	0.52
1:A:111:ARG:HD3	1:A:140:LEU:HB2	1.91	0.52
1:A:91:LEU:HD22	1:A:105:PHE:CE1	2.45	0.52
2:D:51:GLY:H	2:D:53:LYS:HE2	1.74	0.52
1:A:63:VAL:HG12	1:A:138:PRO:HB2	1.92	0.52
2:C:40:GLY:HA3	2:C:136:ILE:HD12	1.90	0.51
1:A:59:ILE:HB	1:A:99:LEU:HD11	1.91	0.51
1:B:88:LEU:HD13	1:B:102:LEU:HD21	1.91	0.51
2:C:47:LEU:HA	2:C:104:ASN:HD21	1.75	0.51
2:C:47:LEU:HB3	2:C:48:PRO:HD2	1.92	0.51
1:A:7:GLN:HB3	3:A:1207:HOH:O	2.10	0.51
2:C:65:VAL:HG11	2:C:111:HIS:HB2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:ARG:HH21	2:C:154:ILE:HD13	1.75	0.51
1:B:60:VAL:HB	3:B:1169:HOH:O	2.09	0.51
1:B:115:ASN:HB2	1:B:138:PRO:HG3	1.93	0.51
2:C:4:VAL:HA	2:C:20:VAL:O	2.10	0.51
2:C:135:ASN:ND2	2:C:137:GLU:HB3	2.21	0.51
2:C:14:LYS:HG2	2:C:15:ASN:H	1.75	0.51
1:A:45:PRO:HA	1:A:163:ASP:C	2.31	0.50
1:A:45:PRO:O	1:A:49:VAL:HB	2.11	0.50
2:C:87:ALA:HA	2:C:123:ASP:O	2.11	0.50
1:B:148:ILE:HA	2:D:92:MET:HE2	1.92	0.50
2:D:30:VAL:O	2:D:42:MET:HA	2.11	0.50
1:A:39:PRO:CD	3:A:1220:HOH:O	2.59	0.50
1:A:73:GLY:HA2	1:A:190:LYS:HG3	1.94	0.49
2:C:21:THR:O	2:C:21:THR:HG23	2.11	0.49
1:A:6:ARG:O	1:A:10:LEU:HD23	2.11	0.49
2:D:35:PRO:O	2:D:38:LYS:HG3	2.11	0.49
1:A:81:THR:OG1	1:A:99:LEU:HD13	2.12	0.49
2:D:104:ASN:O	2:D:108:VAL:HG12	2.12	0.49
1:A:70:ASP:CG	1:A:132:LYS:H	2.16	0.49
2:C:101:GLY:O	2:C:105:VAL:HG23	2.13	0.49
2:C:13:MET:HB3	3:C:1057:HOH:O	2.12	0.49
2:C:20:VAL:HG12	2:C:21:THR:N	2.28	0.49
1:A:39:PRO:HD2	1:A:169:GLU:O	2.13	0.49
2:C:60:TYR:HB2	2:C:63:THR:HG22	1.94	0.49
1:B:149:PHE:CZ	1:B:186:MET:HE3	2.48	0.48
2:D:4:VAL:HG12	2:D:20:VAL:HB	1.95	0.48
2:C:144:ARG:HE	2:C:154:ILE:HG12	1.77	0.48
2:D:94:GLU:HG2	3:D:1294:HOH:O	2.13	0.48
1:A:46:ILE:HA	1:A:49:VAL:CG1	2.43	0.48
2:D:113:LYS:HD2	3:D:1037:HOH:O	2.12	0.48
1:A:45:PRO:O	1:A:49:VAL:N	2.46	0.48
2:C:65:VAL:HG11	2:C:111:HIS:CB	2.44	0.48
2:C:155:LYS:O	2:C:155:LYS:HG3	2.13	0.48
2:D:140:LYS:HG3	2:D:156:GLU:HB3	1.95	0.48
1:B:108:SER:HA	1:B:111:ARG:NH1	2.29	0.48
1:B:91:LEU:HB3	1:B:92:THR:H	1.34	0.48
1:B:65:MET:HB3	1:B:75:VAL:HG23	1.94	0.48
1:B:66:PRO:HG2	1:B:136:LEU:HB2	1.95	0.48
1:A:46:ILE:HA	1:A:49:VAL:HG12	1.94	0.48
1:B:72:GLU:HB2	1:B:193:TYR:CE2	2.49	0.48
2:D:157:ILE:HD13	2:D:157:ILE:H	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:TYR:O	1:B:197:ILE:HG13	2.14	0.47
1:B:45:PRO:HA	1:B:164:GLN:HG2	1.96	0.47
1:A:166:VAL:O	1:A:186:MET:HA	2.14	0.47
2:C:12:VAL:HG22	2:C:41:ALA:HB2	1.96	0.47
2:C:14:LYS:HG2	2:C:15:ASN:N	2.29	0.47
2:D:46:MET:SD	2:D:59:LYS:HE3	2.54	0.47
2:C:90:ALA:HB2	3:C:1330:HOH:O	2.14	0.47
1:B:86:LYS:HG3	1:B:90:ILE:CD1	2.44	0.47
1:A:27:SER:HB2	1:A:34:VAL:HG12	1.97	0.47
1:A:60:VAL:HG21	1:A:78:ILE:CG2	2.42	0.47
1:A:60:VAL:HG22	1:A:61:VAL:N	2.30	0.47
2:C:27:CYS:SG	2:C:46:MET:HA	2.55	0.46
1:B:26:ILE:HD12	1:B:36:ILE:CD1	2.39	0.46
2:D:132:VAL:HA	2:D:142:LEU:O	2.14	0.46
1:A:99:LEU:HD23	1:A:100:LEU:H	1.80	0.46
1:B:167:PHE:HD1	1:B:186:MET:HB3	1.77	0.46
1:A:99:LEU:HD23	1:A:100:LEU:N	2.31	0.46
1:B:86:LYS:CG	1:B:90:ILE:HD13	2.46	0.46
2:C:83:GLU:HB3	2:C:120:LEU:HD22	1.98	0.46
2:C:20:VAL:HG13	2:C:133:GLU:HG2	1.98	0.46
1:B:17:ILE:HD11	3:B:1287:HOH:O	2.15	0.46
2:C:108:VAL:O	2:C:112:LEU:HG	2.16	0.46
2:D:0:HIS:HB3	2:D:2:LYS:NZ	2.31	0.46
1:B:49:VAL:O	1:B:52:ILE:HG22	2.15	0.46
2:D:5:ILE:HD11	2:D:42:MET:HE2	1.98	0.46
1:A:45:PRO:HB3	1:A:163:ASP:CB	2.24	0.45
2:D:14:LYS:O	2:D:136:ILE:HD11	2.17	0.45
1:B:60:VAL:HG21	1:B:145:ILE:HA	1.99	0.45
2:C:53:LYS:HG3	2:C:54:THR:N	2.31	0.45
1:A:60:VAL:O	1:A:142:ILE:HA	2.15	0.45
1:A:179:GLU:CB	1:A:180:PRO:HD2	2.46	0.45
2:C:7:ILE:N	2:C:7:ILE:HD12	2.19	0.45
2:D:128:ARG:HH11	2:D:145:LYS:HE3	1.81	0.45
2:D:33:ARG:HA	2:D:40:GLY:HA2	1.99	0.45
1:B:94:ARG:O	1:B:95:ALA:HB3	2.17	0.45
1:A:162:GLU:HA	1:A:162:GLU:OE1	2.16	0.45
1:A:159:ASP:HA	2:C:46:MET:HE1	1.98	0.45
2:C:48:PRO:O	2:C:61:ALA:HB3	2.17	0.45
2:C:41:ALA:CB	2:C:68:LEU:HG	2.47	0.45
1:A:116:ILE:O	1:A:120:THR:HG23	2.17	0.44
2:C:118:LYS:HA	2:C:118:LYS:HD2	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:ALA:O	2:D:119:LEU:HD23	2.17	0.44
1:A:75:VAL:CG1	1:A:118:CYS:HB3	2.47	0.44
1:B:190:LYS:HB3	1:B:191:PRO:CD	2.44	0.44
2:C:65:VAL:HG13	2:C:66:LYS:N	2.33	0.44
2:C:66:LYS:HD2	3:C:1143:HOH:O	2.17	0.44
1:B:14:ILE:HD13	1:B:125:LEU:HD12	1.99	0.44
2:C:30:VAL:HB	2:C:43:ALA:HB3	1.99	0.44
2:D:120:LEU:HD12	2:D:120:LEU:N	2.32	0.44
1:B:167:PHE:CE1	1:B:186:MET:HB3	2.52	0.44
1:B:136:LEU:HB3	1:B:137:PRO:HD2	1.99	0.44
2:C:70:GLU:O	2:C:74:LYS:HG3	2.18	0.44
1:B:63:VAL:O	1:B:76:LEU:HD12	2.18	0.44
1:B:58:GLU:HG2	1:B:59:ILE:N	2.33	0.44
1:A:85:LYS:O	1:A:87:ILE:N	2.51	0.44
1:B:4:SER:HB3	1:B:7:GLN:HG3	1.99	0.44
1:B:148:ILE:HA	2:D:92:MET:CE	2.48	0.43
1:A:60:VAL:CG2	1:A:78:ILE:HG23	2.46	0.43
1:B:76:LEU:HB3	1:B:186:MET:HG3	1.99	0.43
2:C:98:MET:O	2:C:98:MET:HG3	2.18	0.43
2:C:30:VAL:HG22	2:C:108:VAL:HG11	2.00	0.43
1:A:63:VAL:HA	1:A:139:GLN:O	2.17	0.43
2:D:69:VAL:HG21	2:D:115:PHE:CE2	2.54	0.43
1:A:145:ILE:HG23	1:A:146:SER:N	2.33	0.43
1:B:23:ALA:HB1	1:B:34:VAL:HG13	2.01	0.43
1:B:91:LEU:C	1:B:93:GLY:H	2.22	0.43
2:D:144:ARG:HA	2:D:153:GLU:O	2.18	0.43
1:A:15:GLY:C	1:A:38:VAL:HG21	2.40	0.43
2:D:18:VAL:HA	2:D:134:TYR:O	2.18	0.43
2:C:135:ASN:O	2:C:139:GLY:N	2.51	0.42
1:B:49:VAL:HG12	3:B:1103:HOH:O	2.19	0.42
1:B:62:GLY:N	1:B:141:VAL:O	2.52	0.42
1:B:59:ILE:HD12	2:D:146:VAL:HG12	2.01	0.42
2:C:127:ASN:N	2:C:127:ASN:ND2	2.64	0.42
1:B:94:ARG:C	1:B:96:PRO:CD	2.87	0.42
1:B:98:ASN:O	1:B:102:LEU:HB2	2.20	0.42
1:B:83:VAL:HG22	1:B:181:LEU:HD13	2.02	0.42
1:B:7:GLN:NE2	1:B:198:PHE:CG	2.87	0.42
1:A:145:ILE:HD13	3:A:1363:HOH:O	2.19	0.42
1:B:87:ILE:HG21	1:B:113:ILE:CD1	2.49	0.42
2:C:26:SER:HB2	2:C:101:GLY:CA	2.50	0.42
2:D:26:SER:O	2:D:89:GLY:HA2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:PRO:HA	3:B:1336:HOH:O	2.18	0.42
1:B:61:VAL:HG22	1:B:99:LEU:HD13	2.02	0.42
2:D:66:LYS:HA	2:D:69:VAL:HG22	2.02	0.42
2:D:53:LYS:HG2	2:D:53:LYS:H	1.62	0.42
2:D:100:ILE:HG13	2:D:100:ILE:H	1.54	0.42
1:A:195:VAL:O	1:A:199:GLU:HG2	2.19	0.42
2:C:26:SER:HB2	2:C:101:GLY:HA2	2.02	0.41
1:A:62:GLY:HA2	1:A:77:LEU:O	2.19	0.41
1:A:189:PRO:HB2	1:A:193:TYR:CB	2.50	0.41
1:B:193:TYR:HA	1:B:196:LYS:CB	2.50	0.41
1:A:171:LEU:CB	3:A:1220:HOH:O	2.66	0.41
2:C:4:VAL:HG23	2:C:21:THR:HA	2.03	0.41
1:A:84:VAL:O	1:A:88:LEU:HB2	2.21	0.41
2:D:79:VAL:HA	2:D:82:LEU:HD13	2.02	0.41
2:C:48:PRO:HD3	2:C:104:ASN:ND2	2.35	0.41
1:A:137:PRO:HA	1:A:138:PRO:HD2	1.89	0.41
2:D:143:VAL:HB	2:D:155:LYS:HG3	2.02	0.41
2:C:53:LYS:HG3	2:C:54:THR:H	1.86	0.41
1:B:32:LYS:HG2	3:B:1018:HOH:O	2.20	0.41
1:B:145:ILE:HG23	1:B:146:SER:N	2.36	0.41
2:C:100:ILE:HG12	2:C:100:ILE:H	1.71	0.41
2:C:94:GLU:OE2	2:C:94:GLU:HA	2.21	0.41
2:D:128:ARG:HE	2:D:145:LYS:CE	2.33	0.40
1:A:26:ILE:HD12	1:A:36:ILE:HD11	2.03	0.40
1:B:68:THR:HG22	3:B:1285:HOH:O	2.21	0.40
1:B:104:GLU:HG2	1:B:104:GLU:H	1.55	0.40
1:A:179:GLU:HB3	1:A:180:PRO:HD2	2.03	0.40
2:D:34:ASP:OD1	2:D:77:ALA:HA	2.21	0.40
1:B:65:MET:SD	1:B:75:VAL:CG2	3.10	0.40
2:D:56:LYS:HG2	3:D:1228:HOH:O	2.21	0.40
1:B:46:ILE:HG21	1:B:165:ILE:HD13	2.03	0.40
2:C:31:CYS:O	2:C:84:ALA:HA	2.22	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	187/205 (91%)	169 (90%)	14 (8%)	4 (2%)	9 10
1	B	184/205 (90%)	159 (86%)	19 (10%)	6 (3%)	5 4
2	C	150/159 (94%)	131 (87%)	17 (11%)	2 (1%)	15 21
2	D	150/159 (94%)	137 (91%)	13 (9%)	0	100 100
All	All	671/728 (92%)	596 (89%)	63 (9%)	12 (2%)	11 13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ILE
1	B	91	LEU
1	B	94	ARG
1	B	95	ALA
1	A	163	ASP
1	A	54	LYS
1	A	86	LYS
1	B	126	ALA
1	A	190	LYS
1	B	46	ILE
2	C	74	LYS
2	C	153	GLU

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	162/179 (90%)	146 (90%)	16 (10%)	10 14
1	B	161/179 (90%)	146 (91%)	15 (9%)	11 16
2	C	119/122 (98%)	112 (94%)	7 (6%)	24 38
2	D	117/122 (96%)	104 (89%)	13 (11%)	8 10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	559/602 (93%)	508 (91%)	51 (9%)	12 17

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	40	ASN
1	A	46	ILE
1	A	49	VAL
1	A	59	ILE
1	A	77	LEU
1	A	91	LEU
1	A	99	LEU
1	A	103	ASP
1	A	104	GLU
1	A	140	LEU
1	A	143	ASP
1	A	155	GLU
1	A	156	GLU
1	A	162	GLU
1	A	187	MET
1	B	10	LEU
1	B	31	ASN
1	B	43	ILE
1	B	46	ILE
1	B	49	VAL
1	B	57	GLU
1	B	70	ASP
1	B	75	VAL
1	B	91	LEU
1	B	94	ARG
1	B	97	ASP
1	B	110	LEU
1	B	112	GLU
1	B	139	GLN
1	B	199	GLU
2	C	10	TYR
2	C	78	LYS
2	C	85	LYS
2	C	95	SER
2	C	96	LYS
2	C	98	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	127	ASN
2	D	45	VAL
2	D	54	THR
2	D	80	GLU
2	D	99	ASN
2	D	112	LEU
2	D	118	LYS
2	D	119	LEU
2	D	127	ASN
2	D	130	ARG
2	D	136	ILE
2	D	140	LYS
2	D	141	LEU
2	D	157	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	15	ASN
2	C	104	ASN
2	C	127	ASN
2	C	135	ASN
2	D	99	ASN
2	D	104	ASN

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	193/205 (94%)	0.32	16 (8%) 14 14	15, 50, 94, 115	0
1	B	190/205 (92%)	0.49	25 (13%) 4 4	20, 48, 113, 120	0
2	C	154/159 (96%)	-0.19	4 (2%) 59 58	8, 30, 63, 85	0
2	D	154/159 (96%)	-0.08	5 (3%) 51 51	14, 32, 78, 108	0
All	All	691/728 (94%)	0.16	50 (7%) 18 18	8, 40, 99, 120	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	ILE	7.0
2	D	97	GLY	6.8
1	B	50	ILE	6.6
1	B	96	PRO	5.8
2	C	97	GLY	5.4
1	B	53	ALA	5.1
1	A	156	GLU	5.0
2	C	96	LYS	4.4
1	B	49	VAL	4.4
1	A	101	ASN	4.3
2	C	-1	ALA	4.3
1	A	99	LEU	4.2
1	B	95	ALA	4.1
2	D	98	MET	4.0
1	B	44	VAL	3.8
1	A	105	PHE	3.8
1	B	97	ASP	3.7
1	A	100	LEU	3.7
1	B	94	ARG	3.6
1	B	45	PRO	3.6
1	A	93	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	98	ASN	3.4
1	B	154	ILE	3.4
1	A	51	PHE	3.3
1	A	180	PRO	3.3
2	C	146	VAL	3.3
1	A	50	ILE	3.3
1	B	47	SER	3.2
1	B	52	ILE	3.1
1	B	163	ASP	3.1
1	B	54	LYS	3.1
1	B	181	LEU	3.0
1	B	92	THR	3.0
1	B	167	PHE	2.6
1	A	49	VAL	2.6
1	B	100	LEU	2.5
1	B	89	GLU	2.5
1	A	203	ILE	2.5
1	A	53	ALA	2.5
1	A	181	LEU	2.5
1	A	102	LEU	2.4
2	D	152	LEU	2.4
1	B	165	ILE	2.4
1	A	158	GLU	2.4
2	D	94	GLU	2.3
1	A	45	PRO	2.2
1	B	166	VAL	2.2
1	B	3	ILE	2.1
1	B	51	PHE	2.0
2	D	15	ASN	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 (i)

There are no such residues in this entry.