Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:04 PM GMT

PDB ID	:	1RZG
Title	:	Crystal structure of Human anti-HIV-1 GP120 reactive antibody 412d
Authors	:	Huang, C.C.; Venturi, M.; Majeed, S.; Moore, M.J.; Phogat, S.; Zhang, M.-Y.; Dimitrov, D.S.; Hendrickson, W.A.; Robinson, J.; Sodroski, J.; Wyatt, R.; Choe, H.; Farzan, M.; Kwong, P.D.
Deposited on	:	2003-12-24
Resolution	:	2.00 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:

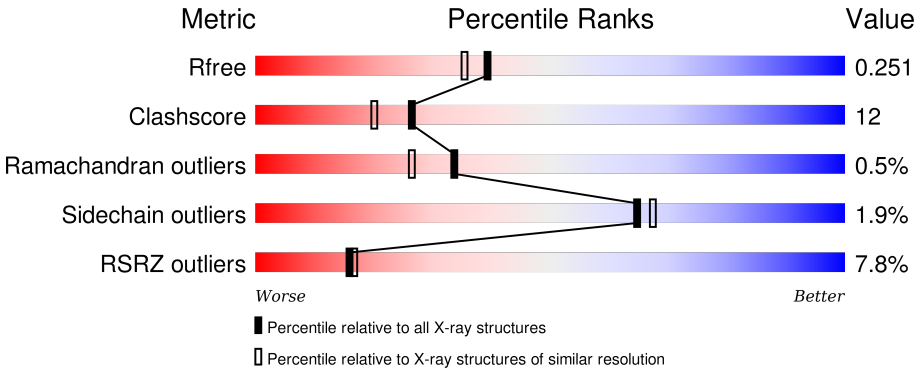
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	231	5% 74% 22% ·
1	C	231	20% 58% 32% · 7%
2	B	214	% 81% 18%
2	D	214	3% 78% 20% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SUC	A	9007	-	-	-	X
3	SUC	C	9006	-	-	-	X
4	ASP	D	9005	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7395 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.

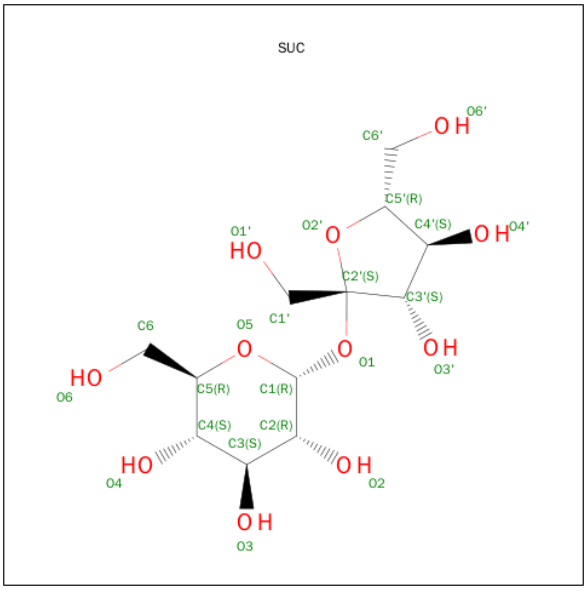
- Molecule 1 is a protein called Fab 412d light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1684	1066	278	332	8			
1	C	214	Total	C	N	O	S	0	0	0
			1617	1029	266	314	8			

- Molecule 2 is a protein called Fab 412d heavy chain.

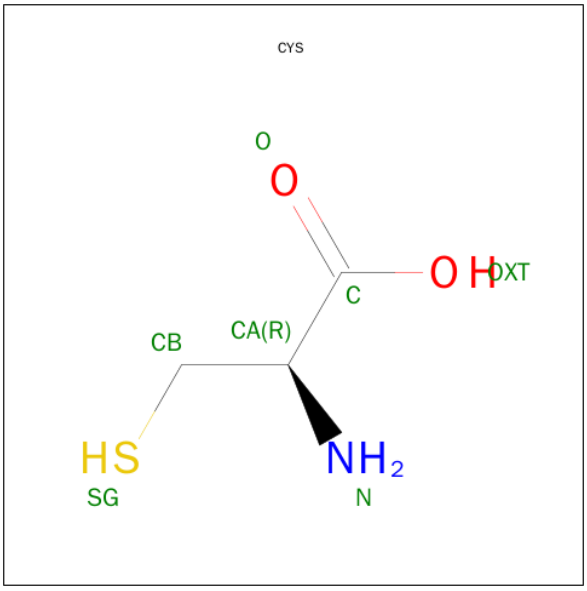
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1642	1024	278	334	6			
2	D	214	Total	C	N	O	S	0	0	0
			1649	1027	279	336	7			

- Molecule 3 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 23 12 11	0	0
3	A	1	Total C O 23 12 11	0	0
3	D	1	Total C O 23 12 11	0	0
3	C	1	Total C O 23 12 11	0	0
3	A	1	Total C O 23 12 11	0	0
3	C	1	Total C O 23 12 11	0	0
3	A	1	Total C O 23 12 11	0	0

- Molecule 4 is CYSTEINE (three-letter code: CYS, ASP) (formula: $C_3H_7NO_2S$, $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	2	Total C N O S 14 7 2 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	176	Total O 176 176	0	0
5	B	193	Total O 193 193	0	0

Continued on next page...

Continued from previous page...

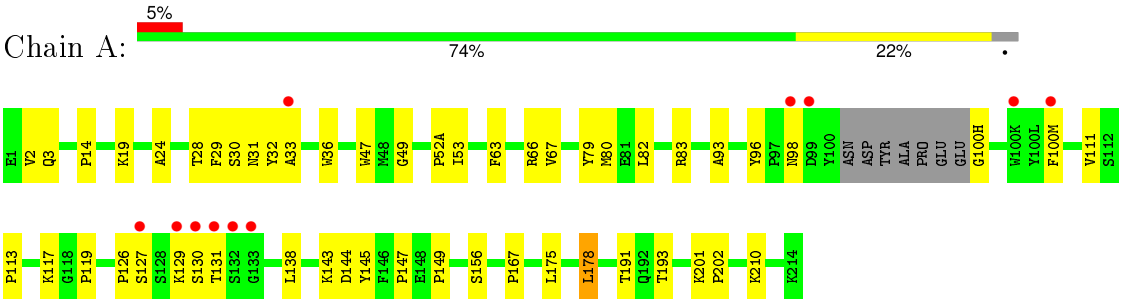
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	103	Total O 103 103	0	0
5	D	156	Total O 156 156	0	0

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.

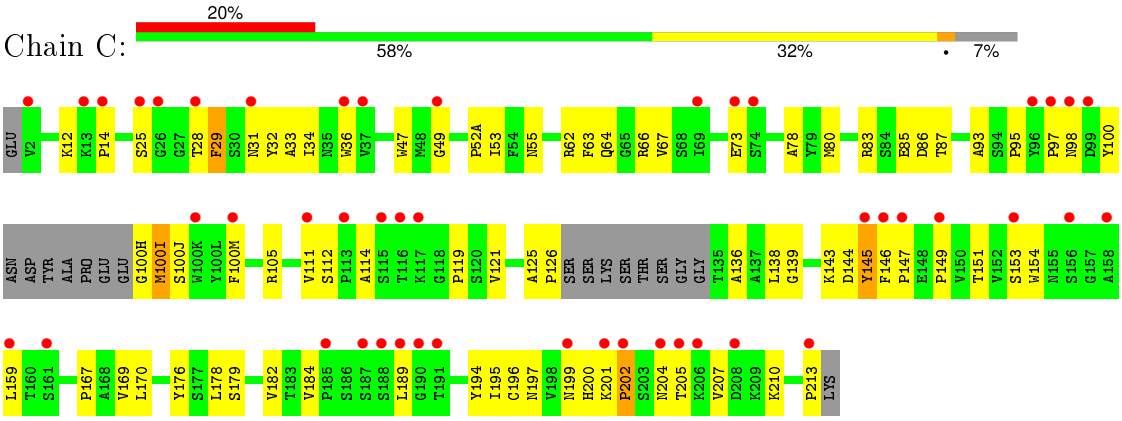
- Molecule 1: Fab 412d light chain

Chain A:



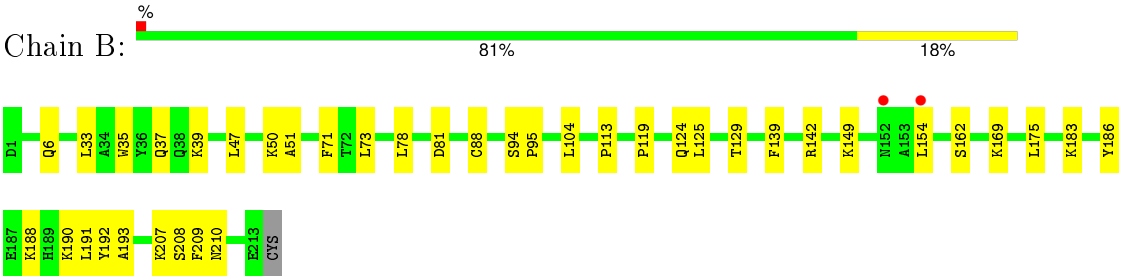
- Molecule 1: Fab 412d light chain

Chain C:



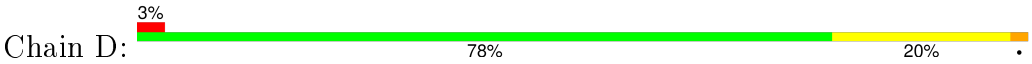
- Molecule 2: Fab 412d heavy chain

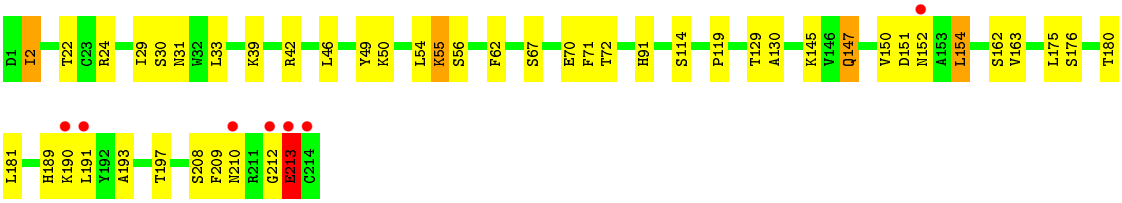
Chain B:



- Molecule 2: Fab 412d heavy chain

Chain D:




D1
I2
T22
G23
R24
I29
S30
N31
W32
L33
K39
R42
L46
Y49
K50
L54
K55
S56
F62
S67
E70
F71
T72
H91
S114
P119
T129
A130
K145
V146
Q147
V150
D151
N152
A153
L154
S162
V163
L175
S176
T180

L181
H189
K190
L191
Y192
A193
T197
S208
F209
N210
R211
G212
E213
C214

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.09Å 89.31Å 85.86Å 90.00° 110.31° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 29.15 – 1.88	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.00) 86.2 (29.15-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 1.88Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.251 0.202 , 0.251	Depositor DCC
R_{free} test set	5758 reflections (10.14%)	DCC
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.0	EDS
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 66703 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7395	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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

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

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	0.34	0/1711	0.67	1/2331 (0.0%)
1	C	0.31	0/1643	0.62	0/2242
2	B	0.33	0/1677	0.65	0/2273
2	D	0.32	0/1684	0.64	1/2281 (0.0%)
All	All	0.33	0/6715	0.65	2/9127 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	33	ALA	N-CA-C	-5.16	97.06	111.00
2	D	114	SER	N-CA-C	-5.02	97.44	111.00

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	1684	0	1639	47	0
1	C	1617	0	1571	60	0
2	B	1642	0	1596	31	0
2	D	1649	0	1600	34	0
3	A	92	0	88	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	46	0	44	2	0
3	D	23	0	22	0	0
4	D	14	0	7	1	0
5	A	176	0	0	4	0
5	B	193	0	0	2	0
5	C	103	0	0	3	0
5	D	156	0	0	2	0
All	All	7395	0	6567	163	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 12.

All (163) 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:129:LYS:HE2	2:B:208:SER:H	1.16	1.03
1:A:126:PRO:HG3	1:A:138:LEU:HB3	1.41	0.97
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.59	0.84
1:C:126:PRO:HG3	1:C:138:LEU:HB3	1.59	0.84
1:C:195:ILE:HG12	1:C:210:LYS:HG2	1.60	0.83
1:C:119:PRO:HD2	1:C:205:THR:HG21	1.64	0.78
2:D:55:LYS:HA	2:D:55:LYS:HE2	1.66	0.78
2:D:193:ALA:HB2	2:D:208:SER:HB3	1.68	0.75
2:D:147:GLN:HG2	2:D:154:LEU:HD21	1.67	0.74
1:A:127:SER:H	1:A:130:SER:HB3	1.52	0.74
1:C:83:ARG:HB2	1:C:85:GLU:HG2	1.69	0.73
1:A:193:THR:HG23	1:A:210:LYS:HE3	1.70	0.72
2:B:188:LYS:HE3	5:B:394:HOH:O	1.91	0.70
1:A:129:LYS:HE3	2:B:207:LYS:HD3	1.76	0.68
1:A:129:LYS:HE2	2:B:208:SER:N	2.00	0.67
1:C:200:HIS:CD2	1:C:202:PRO:HD2	2.30	0.66
2:B:78:LEU:HD11	2:B:104:LEU:HD21	1.77	0.66
1:C:153:SER:HB3	1:C:197:ASN:HB2	1.76	0.65
1:A:67:VAL:HG22	1:A:82:LEU:HD13	1.79	0.65
2:D:46:LEU:HD23	2:D:55:LYS:HD2	1.78	0.65
1:A:2:VAL:HG11	1:A:96:TYR:OH	1.96	0.65
1:C:119:PRO:HG3	1:C:145:TYR:CB	2.27	0.64
1:A:2:VAL:HG13	1:A:2:VAL:O	1.98	0.64
2:B:193:ALA:HB2	2:B:208:SER:HB3	1.78	0.64
1:A:98:ASN:HB2	5:A:9034:HOH:O	1.99	0.63
2:B:190:LYS:HE3	2:B:191:LEU:HD11	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:TYR:HD2	1:C:145:TYR:H	1.47	0.60
1:C:33:ALA:HB3	1:C:95:PRO:HD2	1.85	0.59
1:C:100:TYS:O1	1:C:100(I):MET:HB2	2.01	0.59
2:B:191:LEU:HG	2:B:210:ASN:OD1	2.03	0.59
1:A:30:SER:HB3	1:A:53:ILE:HD12	1.82	0.59
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.84	0.59
1:C:67:VAL:O	3:C:9004:SUC:H2	2.03	0.59
1:A:127:SER:O	1:A:131:THR:HG23	2.03	0.58
1:C:29:PHE:CD2	1:C:52(A):PRO:HB3	2.40	0.57
1:A:178:LEU:C	1:A:178:LEU:HD12	2.25	0.57
1:C:119:PRO:HG3	1:C:145:TYR:HB3	1.87	0.56
1:A:28:THR:OG1	1:A:31:ASN:ND2	2.38	0.56
1:A:100(H):GLY:HA3	3:A:9007:SUC:H2	1.87	0.56
1:C:100(J):SER:HB3	2:D:91:HIS:HD2	1.69	0.56
2:D:30:SER:C	2:D:31:ASN:HD22	2.09	0.56
2:B:142:ARG:HH11	2:B:142:ARG:HG2	1.70	0.56
2:D:193:ALA:CB	2:D:208:SER:HB3	2.34	0.56
1:C:200:HIS:HB3	1:C:205:THR:HB	1.88	0.56
1:C:167:PRO:HD2	2:D:162:SER:OG	2.06	0.55
1:A:14:PRO:HG2	1:A:113:PRO:HG3	1.88	0.55
2:D:212:GLY:O	2:D:213:GLU:C	2.45	0.55
2:B:169:LYS:C	2:B:169:LYS:HD2	2.28	0.55
1:A:129:LYS:HE3	2:B:207:LYS:HA	1.89	0.55
1:C:143:LYS:HG2	1:C:144:ASP:OD2	2.07	0.55
1:C:33:ALA:HB3	1:C:95:PRO:CD	2.38	0.54
2:B:193:ALA:CB	2:B:208:SER:HB3	2.38	0.54
1:C:93:ALA:HB1	1:C:100(M):PHE:HB3	1.91	0.53
1:A:66:ARG:CZ	1:A:83:ARG:HH22	2.22	0.53
2:D:145:LYS:HB3	2:D:197:THR:HB	1.90	0.53
1:A:167:PRO:HD2	2:B:162:SER:OG	2.09	0.53
2:D:55:LYS:HA	2:D:55:LYS:CE	2.38	0.52
1:A:2:VAL:HG13	5:A:9031:HOH:O	2.09	0.52
1:C:126:PRO:CG	1:C:138:LEU:HB3	2.37	0.52
2:B:191:LEU:N	2:B:191:LEU:HD12	2.25	0.52
1:A:93:ALA:HB1	1:A:100(M):PHE:HB3	1.91	0.51
2:B:149:LYS:HG2	2:B:154:LEU:HD23	1.92	0.51
1:A:156:SER:O	1:C:14:PRO:HB2	2.11	0.51
2:B:125:LEU:O	2:B:183:LYS:HD2	2.11	0.50
2:D:119:PRO:HB3	2:D:209:PHE:CE2	2.47	0.50
2:D:31:ASN:N	2:D:31:ASN:HD22	2.10	0.50
1:C:139:GLY:HA2	1:C:154:TRP:CH2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:9004:CYS:HA	5:D:9161:HOH:O	2.11	0.50
1:C:119:PRO:HG3	1:C:145:TYR:HB2	1.92	0.49
2:D:190:LYS:O	2:D:210:ASN:HA	2.12	0.49
1:C:28:THR:OG1	1:C:31:ASN:ND2	2.45	0.49
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.47	0.49
2:D:33:LEU:HD22	2:D:71:PHE:CG	2.47	0.49
1:A:29:PHE:CE2	1:A:52(A):PRO:HB3	2.48	0.49
2:B:6:GLN:HG3	2:B:88:CYS:SG	2.53	0.49
1:C:119:PRO:CB	1:C:145:TYR:HB3	2.43	0.48
1:C:32:TYR:CZ	1:C:97:PRO:HG2	2.47	0.48
1:C:36:TRP:CE2	1:C:80:MET:HB2	2.49	0.48
1:C:105:ARG:NH1	5:C:9063:HOH:O	2.47	0.48
2:D:2:ILE:HD13	2:D:29:ILE:HG22	1.96	0.48
1:C:184:VAL:HG11	1:C:194:TYR:CE2	2.47	0.48
1:A:126:PRO:CG	1:A:138:LEU:HB3	2.29	0.48
2:D:54:LEU:HD21	2:D:62:PHE:O	2.14	0.48
1:A:144:ASP:HB3	1:A:175:LEU:HD13	1.96	0.48
1:A:36:TRP:CE2	1:A:80:MET:HB2	2.49	0.48
2:B:186:TYR:HA	2:B:192:TYR:OH	2.14	0.48
1:C:136:ALA:CB	1:C:189:LEU:HD11	2.44	0.47
2:B:124:GLN:HG2	2:B:129:THR:O	2.14	0.47
1:A:117:LYS:NZ	5:A:9135:HOH:O	2.47	0.47
1:A:83:ARG:C	1:A:111:VAL:HG11	2.35	0.47
2:B:39:LYS:NZ	2:B:81:ASP:OD1	2.47	0.47
2:D:129:THR:HG22	2:D:130:ALA:N	2.31	0.47
1:A:119:PRO:CB	1:A:145:TYR:HB3	2.40	0.46
2:D:55:LYS:NZ	2:D:56:SER:H	2.12	0.46
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.98	0.46
2:B:175:LEU:HD23	2:B:175:LEU:C	2.36	0.46
2:D:39:LYS:HB2	2:D:42:ARG:HD2	1.96	0.46
1:C:202:PRO:HB3	5:C:9080:HOH:O	2.16	0.46
2:D:180:THR:O	2:D:181:LEU:HD23	2.16	0.46
1:A:67:VAL:CG2	1:A:82:LEU:HD13	2.45	0.46
2:D:190:LYS:HD2	2:D:213:GLU:OE2	2.16	0.46
1:A:191:THR:HG23	5:D:9104:HOH:O	2.16	0.46
2:D:31:ASN:ND2	2:D:67:SER:HB2	2.31	0.45
1:A:147:PRO:HB2	5:A:9032:HOH:O	2.16	0.45
1:C:178:LEU:C	1:C:178:LEU:HD23	2.37	0.45
2:D:22:THR:HG22	2:D:72:THR:HG22	1.99	0.45
1:C:126:PRO:HB2	1:C:213:PRO:HB3	1.98	0.45
2:B:50:LYS:O	2:B:51:ALA:HB3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:SER:N	1:A:130:SER:HB3	2.26	0.45
1:A:19:LYS:HE2	1:A:79:TYR:CD2	2.52	0.45
1:C:34:ILE:HG21	1:C:78:ALA:HB3	1.98	0.45
1:A:63:PHE:HB3	1:A:67:VAL:CG2	2.46	0.45
1:A:66:ARG:NE	1:A:83:ARG:HH22	2.15	0.45
1:C:31:ASN:ND2	1:C:98:ASN:O	2.50	0.45
1:C:87:THR:HB	5:C:9101:HOH:O	2.17	0.45
1:C:66:ARG:HH22	1:C:86:ASP:CG	2.19	0.45
2:D:151:ASP:OD2	2:D:189:HIS:HB3	2.16	0.44
1:A:143:LYS:HE2	5:B:230:HOH:O	2.18	0.44
1:A:129:LYS:HE3	2:B:207:LYS:CD	2.47	0.44
1:C:12:LYS:O	1:C:111:VAL:HA	2.17	0.44
1:C:159:LEU:HD21	1:C:182:VAL:HG21	2.00	0.44
1:C:119:PRO:CG	1:C:145:TYR:HB3	2.48	0.43
1:A:31:ASN:ND2	1:A:98:ASN:O	2.50	0.43
1:C:178:LEU:HD23	1:C:179:SER:N	2.33	0.43
1:C:47:TRP:CZ2	1:C:49:GLY:HA2	2.53	0.43
1:C:151:THR:OG1	1:C:199:ASN:HB3	2.18	0.43
1:C:201:LYS:O	1:C:202:PRO:C	2.57	0.43
1:C:63:PHE:O	1:C:67:VAL:HG12	2.19	0.43
1:C:154:TRP:CH2	1:C:196:CYS:HB3	2.54	0.43
2:D:151:ASP:HA	2:D:191:LEU:HB2	2.00	0.43
1:C:119:PRO:HB3	1:C:145:TYR:HB3	2.00	0.43
1:C:86:ASP:O	1:C:87:THR:C	2.57	0.42
2:D:49:TYR:HD1	2:D:50:LYS:HG3	1.83	0.42
2:D:31:ASN:N	2:D:31:ASN:ND2	2.66	0.42
2:D:150:VAL:O	2:D:151:ASP:HB2	2.19	0.42
1:C:169:VAL:O	1:C:176:TYR:HD1	2.02	0.42
1:C:112:SER:C	1:C:114:ALA:H	2.22	0.42
1:A:147:PRO:HD2	1:A:202:PRO:HB3	2.02	0.42
1:C:146:PHE:HA	1:C:147:PRO:HA	1.88	0.42
2:B:94:SER:HA	2:B:95:PRO:C	2.40	0.42
2:B:35:TRP:CE2	2:B:73:LEU:HB2	2.55	0.42
2:D:163:VAL:HG22	2:D:175:LEU:HD12	2.01	0.42
1:A:2:VAL:C	1:A:3:GLN:HG2	2.40	0.41
2:D:175:LEU:HD23	2:D:176:SER:N	2.34	0.41
1:C:31:ASN:CG	1:C:98:ASN:O	2.59	0.41
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.54	0.41
2:B:142:ARG:HG2	2:B:142:ARG:NH1	2.34	0.41
1:A:201:LYS:N	1:A:202:PRO:CD	2.83	0.41
1:C:170:LEU:HD13	1:C:176:TYR:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ALA:HA	1:C:126:PRO:HD3	1.82	0.41
1:A:66:ARG:CZ	1:A:83:ARG:NH2	2.84	0.41
2:B:119:PRO:HB3	2:B:209:PHE:CZ	2.55	0.41
1:C:53:ILE:HD12	1:C:73:GLU:OE2	2.19	0.41
2:D:193:ALA:HB2	2:D:208:SER:CB	2.45	0.41
2:D:31:ASN:HD21	2:D:67:SER:HB2	1.85	0.41
1:C:55:ASN:HA	1:C:55:ASN:HD22	1.68	0.41
1:C:100(H):GLY:O	1:C:100(I):MET:C	2.58	0.41
2:D:24:ARG:HG2	2:D:70:GLU:OE2	2.20	0.41
1:A:24:ALA:HB1	1:A:32:TYR:CZ	2.55	0.40
1:C:64:GLN:HA	3:C:9004:SUC:O2	2.21	0.40
1:C:145:TYR:CD2	1:C:145:TYR:N	2.89	0.40
1:A:129:LYS:CE	2:B:207:LYS:HA	2.51	0.40
1:C:121:VAL:HG21	1:C:207:VAL:CG1	2.51	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	220/231 (95%)	211 (96%)	9 (4%)	0	100 100
1	C	208/231 (90%)	180 (86%)	26 (12%)	2 (1%)	19 11
2	B	211/214 (99%)	202 (96%)	9 (4%)	0	100 100
2	D	212/214 (99%)	203 (96%)	7 (3%)	2 (1%)	21 13
All	All	851/890 (96%)	796 (94%)	51 (6%)	4 (0%)	34 26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	25	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	100(I)	MET
2	D	213	GLU
2	D	2	ILE

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	187/193 (97%)	185 (99%)	2 (1%)	80 83
1	C	179/193 (93%)	173 (97%)	6 (3%)	44 41
2	B	188/189 (100%)	188 (100%)	0	100 100
2	D	189/189 (100%)	184 (97%)	5 (3%)	54 54
All	All	743/764 (97%)	730 (98%)	13 (2%)	65 71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	PRO
1	A	178	LEU
1	C	29	PHE
1	C	62	ARG
1	C	145	TYR
1	C	149	PRO
1	C	202	PRO
1	C	204	ASN
2	D	55	LYS
2	D	147	GLN
2	D	152	ASN
2	D	154	LEU
2	D	213	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	55	ASN
1	A	58	HIS
2	B	3	GLN
2	B	27	GLN
2	B	31	ASN
2	B	79	GLN
2	B	91	HIS
1	C	31	ASN
1	C	55	ASN
2	D	31	ASN
2	D	91	HIS
2	D	138	ASN
2	D	210	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TYS	A	100	1	15,16,17	2.23	2 (13%)	16,22,24	1.43	1 (6%)
1	TYS	C	100	1	15,16,17	2.24	2 (13%)	16,22,24	0.78	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TYS	A	100	1	-	0/9/11/13	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TYS	C	100	1	-	0/9/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	TYS	OH-S	-8.06	1.48	1.63
1	C	100	TYS	OH-S	-8.00	1.48	1.63
1	C	100	TYS	OH-CZ	-2.79	1.38	1.42
1	A	100	TYS	OH-CZ	-2.39	1.38	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	100	TYS	CZ-OH-S	2.33	122.48	118.52
1	A	100	TYS	CZ-OH-S	5.31	127.56	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	100	TYS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SUC	A	9001	-	24,24,24	0.97	1 (4%)	36,36,36	0.99	3 (8%)
3	SUC	A	9002	-	24,24,24	1.00	1 (4%)	36,36,36	0.98	3 (8%)
3	SUC	A	9005	-	24,24,24	1.01	1 (4%)	36,36,36	0.90	2 (5%)
3	SUC	A	9007	-	24,24,24	1.02	1 (4%)	36,36,36	0.98	2 (5%)
3	SUC	C	9004	-	24,24,24	0.97	1 (4%)	36,36,36	0.94	2 (5%)
3	SUC	C	9006	-	24,24,24	1.04	1 (4%)	36,36,36	0.99	2 (5%)
3	SUC	D	9003	-	24,24,24	0.99	1 (4%)	36,36,36	0.99	2 (5%)
4	CYS	D	9004	2,4	4,5,6	0.53	0	3,5,7	1.31	0
4	ASP	D	9005	4	3,7,8	0.75	0	1,8,10	2.89	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SUC	A	9001	-	-	0/12/51/51	0/2/2/2
3	SUC	A	9002	-	-	0/12/51/51	0/2/2/2
3	SUC	A	9005	-	-	0/12/51/51	0/2/2/2
3	SUC	A	9007	-	-	0/12/51/51	0/2/2/2
3	SUC	C	9004	-	-	0/12/51/51	0/2/2/2
3	SUC	C	9006	-	-	0/12/51/51	0/2/2/2
3	SUC	D	9003	-	-	0/12/51/51	0/2/2/2
4	CYS	D	9004	2,4	-	0/1/4/6	0/0/0/0
4	ASP	D	9005	4	-	0/2/6/8	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	9004	SUC	C4-C5	2.65	1.58	1.53
3	D	9003	SUC	C4-C5	2.71	1.58	1.53
3	A	9007	SUC	C4-C5	2.74	1.58	1.53
3	A	9001	SUC	C4-C5	2.76	1.58	1.53
3	A	9005	SUC	C4-C5	2.82	1.59	1.53
3	A	9002	SUC	C4-C5	2.84	1.59	1.53
3	C	9006	SUC	C4-C5	2.89	1.59	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	9005	ASP	O-C-CA	-2.89	117.95	125.49
3	A	9001	SUC	O2'-C2'-C1'	2.14	113.80	107.98
3	A	9002	SUC	O2'-C2'-C1'	2.15	113.83	107.98
3	A	9005	SUC	C6-C5-C4	2.16	118.33	113.02
3	C	9004	SUC	C6-C5-C4	2.19	118.42	113.02
3	A	9001	SUC	C6-C5-C4	2.23	118.53	113.02
3	A	9002	SUC	C6-C5-C4	2.30	118.69	113.02
3	A	9007	SUC	C6-C5-C4	2.35	118.82	113.02
3	D	9003	SUC	C6-C5-C4	2.37	118.85	113.02
3	C	9006	SUC	C6-C5-C4	2.40	118.95	113.02
3	A	9002	SUC	C1-O5-C5	2.46	118.52	113.75
3	C	9004	SUC	C1-O5-C5	2.47	118.54	113.75
3	A	9005	SUC	C1-O5-C5	2.52	118.64	113.75
3	C	9006	SUC	C1-O5-C5	2.63	118.85	113.75
3	A	9007	SUC	C1-O5-C5	2.65	118.89	113.75
3	A	9001	SUC	C1-O5-C5	2.71	119.01	113.75
3	D	9003	SUC	C1-O5-C5	2.72	119.02	113.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9007	SUC	1	0
3	C	9004	SUC	2	0
4	D	9004	CYS	1	0

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^{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	223/231 (96%)	0.07	11 (4%) 33 35	17, 29, 50, 72	0
1	C	213/231 (92%)	1.01	47 (22%) 1 1	22, 45, 67, 76	0
2	B	213/214 (99%)	-0.23	2 (0%) 85 86	16, 27, 42, 65	0
2	D	214/214 (100%)	-0.07	7 (3%) 50 51	22, 32, 49, 87	0
All	All	863/890 (96%)	0.19	67 (7%) 16 17	16, 32, 58, 87	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	ASN	7.2
1	C	99	ASP	5.7
1	A	129	LYS	5.5
1	A	130	SER	5.5
2	D	214	CYS	5.2
1	C	25	SER	5.2
1	C	191	THR	5.1
1	A	132	SER	5.0
1	C	201	LYS	4.7
1	C	113	PRO	4.7
1	A	131	THR	4.7
2	D	213	GLU	4.5
1	C	74	SER	4.2
1	A	99	ASP	4.1
2	D	212	GLY	4.0
1	A	133	GLY	3.9
1	C	149	PRO	3.8
1	C	187	SER	3.6
1	C	36	TRP	3.4
1	C	115	SER	3.4
2	D	191	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	26	GLY	3.3
1	C	28	THR	3.3
1	C	189	LEU	3.2
1	C	204	ASN	3.1
1	C	147	PRO	3.1
1	C	205	THR	3.0
1	C	206	LYS	3.0
1	C	116	THR	3.0
1	A	100(M)	PHE	3.0
2	B	154	LEU	3.0
1	C	202	PRO	2.9
1	C	156	SER	2.9
1	C	97	PRO	2.9
1	C	159	LEU	2.9
1	C	96	TYR	2.8
1	C	208	ASP	2.8
1	C	199	ASN	2.8
1	C	2	VAL	2.8
1	C	158	ALA	2.7
1	C	190	GLY	2.7
1	C	100(M)	PHE	2.7
1	C	146	PHE	2.7
1	A	100(K)	TRP	2.6
1	C	49	GLY	2.6
1	C	37	VAL	2.6
1	C	188	SER	2.5
2	D	190	LYS	2.5
1	C	69	ILE	2.5
1	C	100(K)	TRP	2.4
1	C	185	PRO	2.3
1	C	117	LYS	2.3
1	C	31	ASN	2.3
1	C	73	GLU	2.3
1	C	111	VAL	2.3
1	C	153	SER	2.2
1	A	33	ALA	2.2
1	A	98	ASN	2.2
1	C	213	PRO	2.2
1	C	145	TYR	2.1
1	C	161	SER	2.1
2	D	152	ASN	2.1
1	A	127	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	13	LYS	2.1
1	C	14	PRO	2.1
2	D	210	ASN	2.0
2	B	152	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	TYS	A	100	16/17	0.73	0.43	-	72,81,89,89	0
1	TYS	C	100	16/17	0.84	0.51	-	78,86,95,96	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ASP	D	9005	8/9	0.62	0.20	3.60	86,86,87,87	0
3	SUC	C	9006	23/23	0.67	0.25	2.83	67,71,73,73	0
3	SUC	A	9007	23/23	0.58	0.23	2.15	82,84,86,86	0
3	SUC	A	9005	23/23	0.85	0.14	1.43	30,36,40,42	0
3	SUC	D	9003	23/23	0.84	0.17	1.03	42,46,48,49	0
3	SUC	C	9004	23/23	0.89	0.12	0.10	43,46,48,49	0
3	SUC	A	9001	23/23	0.94	0.08	-0.51	26,28,32,34	0
3	SUC	A	9002	23/23	0.91	0.10	-0.62	22,30,33,36	0
4	CYS	D	9004	6/7	0.54	0.27	-	87,87,87,89	0

6.5 Other polymers (i)

There are no such residues in this entry.