WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2017 – 01:37 AM EST

PDB ID	:	5T08
Title	:	Crystal structure of H6 hemagglutinin G225D mutant from Taiwan (2013) H6N1 influenza virus
Authors	:	Wilson, I.A.; Tzarum, N.; Zhu, X.
Deposited on	:	unknown
Resolution	:	2.19 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

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 2.19 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.
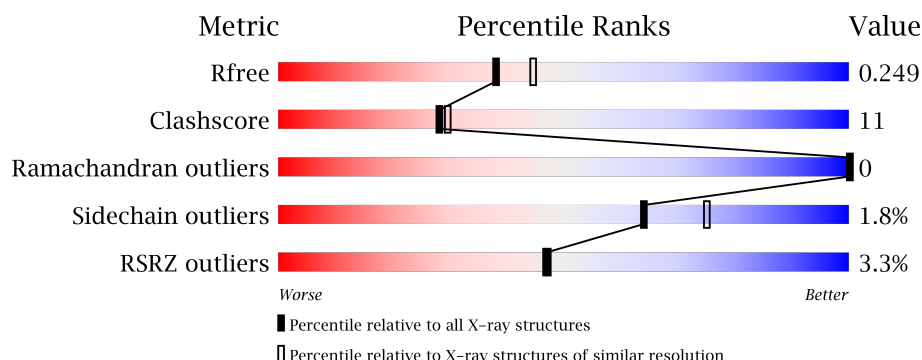
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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	333	2% / 72% / 26% ··
1	C	333	4% / 78% / 19% ··
1	E	333	2% / 70% / 26% ··
2	B	180	2% / 75% / 21% ··
2	D	180	6% / 82% / 14% ·

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Mol	Chain	Length	Quality of chain
2	F	180	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12376 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total 2604	C 1650	N 443	O 498	S 13	0	0	0
1	C	325	Total 2566	C 1627	N 436	O 490	S 13	0	0	0
1	E	325	Total 2569	C 1629	N 437	O 490	S 13	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ASP	GLY	engineered mutation	UNP A0A0J9X268
C	225	ASP	GLY	engineered mutation	UNP A0A0J9X268
E	225	ASP	GLY	engineered mutation	UNP A0A0J9X268

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total 1393	C 868	N 244	O 274	S 7	0	0	0
2	D	173	Total 1393	C 868	N 244	O 274	S 7	0	0	0
2	F	172	Total 1385	C 862	N 243	O 273	S 7	0	0	0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5				0	0
3	A	1	Total C N O 14 8 1 5				0	0
3	E	1	Total C N O 14 8 1 5				0	0
3	E	1	Total C N O 14 8 1 5				0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total O 71 71		0	0
4	B	64	Total O 64 64		0	0
4	C	85	Total O 85 85		0	0
4	D	43	Total O 43 43		0	0
4	E	89	Total O 89 89		0	0
4	F	58	Total O 58 58		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 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: Hemagglutinin

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K265 L274 E277 N278 C279 Q284 T285 I286 T287 G288 V289 L290 R291 T292 N293 K294 T295 F296 Q297 N298 V299 S300 P301 C307 P308 K309 Y310 L322 R323 Q327 ILE ALA THR ARG

• Molecule 2: Hemagglutinin HA2 chain

Chain B:

2%

75%   21%

G1 I2 F3 E11 G12 G13 W14 I18 D19 G20 W21 Y22 H25 H26 E27 Q30 G31 S32 A36 E64 D67 R75 L89 T93 Y94 E97 L98 L99 N104 E105 L108 N135 E139 F140 W141 D145 C148 S151 Y157 D158 Y159

P160 Q163 K167 R170 Q171 G172 I173 GLU GLY ARG LEU VAL PRO ARG

• Molecule 2: Hemagglutinin HA2 chain

Chain D:

6%

82%   14%

G1 I2 F3 G4 F9 I10 M17 Y22 G23 Y24 H25 H26 E27 G33 Y34 R38 K58 E64 R75 L98 E105 A113 L118 L133 G134 N135 E139 D145 C148 Q163 K164 K167 L168 N169 R170 Q171 G172 I173 GLU GLY ARG LEU

VAL PRO ARG

• Molecule 2: Hemagglutinin HA2 chain

Chain F:

5%

74%   21%

G1 I2 F3 F9 W14 M17 I18 D19 G20 W21 Y22 G23 S29 Q30 R38 Q42 S54 I55 I56 N57 K58 M59 Q62 F70 E74 R75 R76 I77 E97 L98 L99 H111 D112 A113 V122 G134 N135 W141 H142 K143 C144 D145 N146 E147 C148

D158 Y159 P160 K161 Y162 L168 Q171 G172 ILE GLU GLY ARG LEU VAL PRO ARG

4   Data and refinement statistics (i)

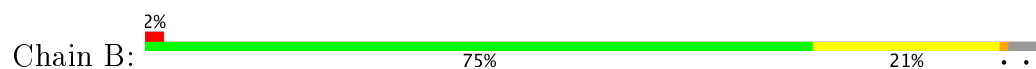| Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	185.06Å 98.36Å 133.24Å 90.00° 126.48° 90.00°	Depositor
Resolution (Å)	49.34 – 2.19 49.34 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.34-2.19) 93.4 (49.34-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.215 , 0.250 0.214 , 0.249	Depositor DCC
R_{free} test set	4587 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.5	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12376	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.56	3/2666 (0.1%)	0.74	3/3628 (0.1%)
1	C	0.60	4/2626 (0.2%)	0.73	4/3572 (0.1%)
1	E	0.55	0/2630	0.74	4/3576 (0.1%)
2	B	0.54	0/1421	0.66	1/1913 (0.1%)
2	D	0.55	0/1421	0.68	1/1913 (0.1%)
2	F	0.52	0/1413	0.69	1/1902 (0.1%)
All	All	0.56	7/12177 (0.1%)	0.71	14/16504 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	F	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	LYS	CE-NZ	6.55	1.65	1.49
1	C	4	LYS	CE-NZ	6.20	1.64	1.49
1	A	4	LYS	CD-CE	6.20	1.66	1.51
1	C	4	LYS	CD-CE	6.15	1.66	1.51
1	C	104	LYS	CE-NZ	6.07	1.64	1.49
1	A	4	LYS	CG-CD	5.12	1.69	1.52
1	C	4	LYS	CG-CD	5.07	1.69	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LYS	CD-CE-NZ	9.61	133.81	111.70
2	D	1	GLY	N-CA-C	-8.55	91.72	113.10
1	C	4	LYS	CD-CE-NZ	8.54	131.35	111.70
2	B	1	GLY	N-CA-C	-8.26	92.46	113.10
2	F	1	GLY	N-CA-C	-8.13	92.77	113.10
1	E	74	GLY	N-CA-C	7.47	131.77	113.10
1	C	71	LEU	CA-CB-CG	6.64	130.58	115.30
1	E	186	LEU	CA-CB-CG	6.15	129.44	115.30
1	C	71	LEU	C-N-CA	6.03	136.78	121.70
1	A	108	GLY	N-CA-C	-5.82	98.55	113.10
1	A	172	GLY	N-CA-C	5.78	127.55	113.10
1	E	195	TYR	C-N-CA	-5.39	110.97	122.30
1	E	71	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	71	LEU	CA-C-N	5.05	128.31	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	71	LEU	Peptide
2	F	134	GLY	Peptide

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	2604	0	2552	81	0
1	C	2566	0	2510	60	0
1	E	2569	0	2515	69	0
2	B	1393	0	1309	28	0
2	D	1393	0	1309	27	0
2	F	1385	0	1298	28	0
3	A	28	0	26	0	0
3	E	28	0	26	0	0
4	A	71	0	0	4	0
4	B	64	0	0	1	0
4	C	85	0	0	10	0
4	D	43	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	89	0	0	3	0
4	F	58	0	0	3	0
All	All	12376	0	11545	261	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 11.

All (261) 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:C:156:THR:O	1:C:159:ALA:CB	1.72	1.37
1:C:156:THR:O	1:C:159:ALA:HB1	1.32	1.14
1:E:307:CYS:O	2:F:62:GLN:NE2	1.95	0.98
1:C:4:LYS:NZ	2:D:25:HIS:HE1	1.61	0.96
2:B:30:GLN:HE21	2:B:145:ASP:HB2	1.34	0.93
1:C:156:THR:O	1:C:159:ALA:HB2	1.70	0.90
1:A:111:GLU:HB2	1:A:263:THR:HB	1.55	0.88
1:C:157:ASP:C	1:C:159:ALA:HB2	1.94	0.86
1:C:266:LYS:NZ	2:D:64:GLU:OE1	2.10	0.83
1:C:158:SER:N	1:C:159:ALA:HB2	1.93	0.83
1:A:290:LEU:HD11	1:A:297:GLN:HG3	1.61	0.82
1:A:263:THR:OG1	1:A:265:LYS:HG2	1.78	0.82
2:B:30:GLN:NE2	2:B:145:ASP:HB2	1.95	0.82
2:F:17:MET:SD	2:F:23:GLY:HA3	2.20	0.81
1:A:297:GLN:NE2	1:A:300:SER:H	1.81	0.78
2:F:142:HIS:O	4:F:201:HOH:O	2.02	0.77
1:C:53:ASP:OD2	4:C:401:HOH:O	2.03	0.76
1:C:171:THR:N	4:C:405:HOH:O	2.18	0.76
1:A:119:PHE:O	4:A:501:HOH:O	2.02	0.76
1:A:297:GLN:HE21	1:A:299:VAL:N	1.83	0.75
1:A:242:THR:OG1	4:A:502:HOH:O	2.04	0.75
1:C:4:LYS:HZ1	2:D:25:HIS:HE1	1.32	0.75
1:E:285:THR:HG22	1:E:287:THR:H	1.51	0.73
1:E:221:PRO:O	1:E:229:ARG:NH2	2.22	0.72
1:C:286:ILE:O	4:C:402:HOH:O	2.07	0.72
2:F:143:LYS:O	4:F:202:HOH:O	2.07	0.71
1:C:4:LYS:NZ	2:D:25:HIS:CE1	2.52	0.70
1:A:156:THR:HG23	1:A:158:SER:H	1.56	0.70
1:E:186:LEU:HD13	1:E:227:ARG:HB2	1.72	0.70
1:C:160:THR:O	4:C:403:HOH:O	2.09	0.70
1:A:68:LYS:HE2	1:A:138:PRO:HG2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:CD1	1:A:297:GLN:HG3	2.22	0.70
1:A:128:ASP:OD2	1:A:131:ARG:HG2	1.91	0.69
1:E:109:SER:HB3	1:E:110:GLY:O	1.90	0.69
1:E:13:ASN:OD1	4:E:501:HOH:O	2.09	0.69
1:C:173:THR:HG23	1:C:174:GLN:HG3	1.73	0.69
2:D:133:LEU:HD11	2:D:139:GLU:HB2	1.75	0.68
1:C:271:LYS:NZ	4:C:406:HOH:O	2.27	0.68
1:A:79:SER:HA	1:A:265:LYS:HE2	1.76	0.67
1:C:20:THR:HG23	2:D:105:GLU:HB2	1.77	0.66
1:C:20:THR:HG22	1:C:22:LEU:H	1.60	0.65
1:C:314:GLU:OE2	4:C:404:HOH:O	2.13	0.65
1:A:199:ASP:O	1:A:248:ASN:ND2	2.29	0.65
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.78	0.65
2:B:75:ARG:N	1:E:102:GLU:OE2	2.25	0.64
1:A:266:LYS:O	1:A:304:ILE:CD1	2.47	0.63
1:C:4:LYS:HG2	2:D:27:GLU:HB3	1.81	0.62
1:E:285:THR:HB	1:E:288:GLY:O	1.98	0.62
1:A:46:ILE:HD11	1:A:304:ILE:HG23	1.81	0.62
1:E:112:ARG:HB3	1:E:261:VAL:CG1	2.31	0.61
1:E:285:THR:HG23	1:E:300:SER:HB3	1.81	0.61
2:D:34:TYR:OH	4:D:201:HOH:O	2.15	0.61
1:E:107:ILE:O	1:E:109:SER:HA	2.00	0.60
1:A:264:ASN:N	1:A:264:ASN:OD1	2.32	0.60
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.83	0.60
1:E:118:MET:HE2	1:E:257:ALA:HB2	1.84	0.60
1:E:7:ILE:HD11	2:F:122:VAL:HG21	1.84	0.60
1:A:297:GLN:NE2	1:A:310:TYR:HD1	2.01	0.59
2:B:148:CYS:O	2:B:151:SER:HB3	2.01	0.59
1:A:45:LYS:O	4:A:503:HOH:O	2.17	0.59
1:A:39:LYS:HD3	1:A:299:VAL:HG13	1.85	0.59
1:A:76:GLN:O	1:A:112:ARG:HB2	2.03	0.58
1:C:4:LYS:HZ1	2:D:25:HIS:CE1	2.19	0.58
1:A:141:THR:HG23	1:A:142:ILE:HG13	1.85	0.58
1:A:297:GLN:HE22	1:A:300:SER:H	1.51	0.58
2:D:145:ASP:HB3	2:D:148:CYS:H	1.69	0.57
1:C:158:SER:HB2	1:C:159:ALA:HA	1.86	0.57
1:E:118:MET:HE1	1:E:178:TYR:HB2	1.85	0.57
1:A:297:GLN:HE21	1:A:299:VAL:H	1.49	0.56
1:A:266:LYS:O	1:A:304:ILE:HD12	2.04	0.56
1:A:70:ASP:O	1:A:73:LEU:HB2	2.06	0.56
1:C:20:THR:HG22	1:C:22:LEU:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLN:HE22	1:A:310:TYR:HD1	1.52	0.56
1:C:4:LYS:HZ2	2:D:25:HIS:CE1	2.24	0.55
1:E:295:THR:HG21	2:F:56:ILE:HG12	1.88	0.55
1:E:201:TYR:HE1	1:E:248:ASN:HD22	1.52	0.55
1:C:328:ILE:O	1:C:329:ALA:HB2	2.06	0.55
1:A:121:LYS:HD3	1:A:129:THR:HB	1.89	0.55
1:E:110:GLY:N	4:E:507:HOH:O	2.38	0.55
1:A:201:TYR:CD1	1:A:248:ASN:HB2	2.42	0.55
1:A:151:VAL:HG23	1:A:255:TRP:HB2	1.88	0.54
2:B:98:LEU:HD21	2:F:99:LEU:HD13	1.88	0.54
1:E:158:SER:O	1:E:159:ALA:HB3	2.06	0.54
2:B:2:ILE:HG23	2:B:3:PHE:N	2.22	0.54
1:A:207:GLU:OE1	1:A:241:GLU:HG2	2.07	0.54
1:A:201:TYR:CE1	1:A:248:ASN:HB2	2.43	0.54
1:C:67:PRO:HG3	1:C:146:PHE:O	2.07	0.54
1:A:266:LYS:HE3	2:B:64:GLU:OE1	2.08	0.54
2:B:11:GLU:HG3	2:B:135:ASN:OD1	2.08	0.54
1:C:69:CYS:O	1:C:72:LEU:HB3	2.08	0.54
2:B:151:SER:OG	2:B:157:TYR:HA	2.08	0.53
1:A:187:ASP:HB3	1:A:190:VAL:H	1.74	0.53
1:C:25:ASN:ND2	4:C:409:HOH:O	2.40	0.53
2:D:167:LYS:HA	2:D:170:ARG:HE	1.74	0.53
1:E:290:LEU:HD21	1:E:299:VAL:HG21	1.91	0.53
1:A:227:ARG:NH2	1:E:244:ASN:HD21	2.07	0.53
1:A:102:GLU:OE2	2:D:75:ARG:N	2.33	0.52
1:E:155:LYS:HB2	1:E:194:LEU:O	2.10	0.52
1:E:46:ILE:HD11	1:E:284:GLN:HB2	1.92	0.52
1:A:227:ARG:HH21	1:E:244:ASN:HD21	1.58	0.52
2:F:3:PHE:CE2	2:F:113:ALA:HB2	2.44	0.52
2:F:2:ILE:HG23	2:F:3:PHE:N	2.25	0.52
1:A:78:TRP:CZ3	1:A:112:ARG:HA	2.44	0.52
1:E:95:GLY:HA3	1:E:230:ILE:O	2.08	0.52
1:E:42:ARG:NH2	1:E:279:CYS:SG	2.83	0.51
1:A:266:LYS:O	1:A:304:ILE:HD11	2.10	0.51
1:C:40:GLU:HB2	1:C:289:VAL:HB	1.92	0.51
2:F:158:ASP:OD1	2:F:160:PRO:HG2	2.11	0.51
1:C:157:ASP:N	1:C:157:ASP:OD1	2.40	0.50
2:D:25:HIS:HD2	2:D:33:GLY:O	1.95	0.50
1:C:121:LYS:HG2	1:C:129:THR:HB	1.93	0.50
1:E:200:LYS:NZ	4:E:509:HOH:O	2.44	0.50
1:E:285:THR:HG22	1:E:287:THR:N	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:LYS:HE3	2:F:97:GLU:HB3	1.94	0.50
2:D:17:MET:SD	2:D:23:GLY:HA3	2.51	0.49
1:E:43:PHE:CE2	1:E:274:LEU:HB2	2.47	0.49
1:A:283:CYS:SG	1:A:290:LEU:HB2	2.52	0.49
1:A:201:TYR:H	1:A:248:ASN:HB3	1.77	0.49
1:A:134:THR:HG23	1:A:137:CYS:H	1.77	0.49
2:D:2:ILE:HG23	2:D:3:PHE:N	2.26	0.49
1:A:118:MET:HE2	1:A:257:ALA:HB2	1.94	0.49
1:E:23:GLU:CD	1:E:323:ARG:HH22	2.15	0.49
2:F:162:TYR:OH	4:F:203:HOH:O	2.18	0.49
1:E:74:GLY:HA2	1:E:115:ARG:HD3	1.94	0.49
1:A:109:SER:N	1:A:110:GLY:HA3	2.27	0.48
1:E:64:LEU:O	1:E:147:TYR:HB3	2.13	0.48
1:E:128:ASP:OD2	1:E:131:ARG:HG3	2.13	0.48
1:E:37:ASN:HA	1:E:298:ASN:ND2	2.28	0.48
1:E:10:HIS:HB2	2:F:20:GLY:O	2.13	0.48
1:E:59:ILE:O	1:E:63:ILE:HG13	2.12	0.48
1:C:297:GLN:HG2	1:C:308:PRO:HG2	1.96	0.47
1:E:49:LYS:HB3	1:E:79:SER:HB3	1.96	0.47
2:F:38:ARG:NH1	2:F:42:GLN:OE1	2.38	0.47
2:F:74:GLU:HB3	2:F:77:ILE:HD11	1.94	0.47
1:E:277:GLU:C	1:E:279:CYS:H	2.18	0.47
1:E:186:LEU:HD13	1:E:227:ARG:CB	2.43	0.47
1:E:67:PRO:HG3	1:E:146:PHE:O	2.14	0.47
2:F:70:PHE:CD1	2:F:77:ILE:HD12	2.50	0.47
2:F:38:ARG:NH1	2:F:42:GLN:HB2	2.30	0.47
1:E:59:ILE:HG13	1:E:83:GLU:OE2	2.14	0.46
1:E:37:ASN:HA	1:E:298:ASN:HD21	1.81	0.46
1:C:165:LYS:HG2	1:C:246:GLU:HG3	1.96	0.46
1:A:95:GLY:HA3	1:A:230:ILE:O	2.15	0.46
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.50	0.46
1:E:322:LEU:HB3	2:F:111:HIS:CG	2.51	0.46
2:D:145:ASP:N	2:D:148:CYS:HB3	2.30	0.46
1:E:187:ASP:HB3	1:E:189:THR:H	1.80	0.46
2:D:3:PHE:CE2	2:D:113:ALA:HB2	2.51	0.46
1:E:285:THR:HG21	1:E:299:VAL:HG12	1.97	0.46
2:F:145:ASP:N	2:F:148:CYS:HB3	2.31	0.46
1:A:265:LYS:HA	4:A:535:HOH:O	2.16	0.45
2:F:2:ILE:HG23	2:F:3:PHE:CD2	2.51	0.45
1:A:4:LYS:NZ	2:B:25:HIS:NE2	2.51	0.45
1:C:200:LYS:HD2	1:C:249:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:PHE:O	2:D:135:ASN:HA	2.16	0.45
1:C:175:PRO:HD2	1:C:260:PHE:O	2.16	0.45
1:A:63:ILE:O	1:A:149:ASN:ND2	2.49	0.45
2:B:2:ILE:HG12	2:B:2:ILE:O	2.15	0.45
1:C:156:THR:C	1:C:159:ALA:CB	2.73	0.45
1:E:112:ARG:HB3	1:E:261:VAL:HG11	1.98	0.45
2:B:93:THR:O	2:B:97:GLU:HG3	2.16	0.45
1:C:158:SER:N	1:C:159:ALA:CB	2.73	0.45
1:C:95:GLY:HA3	1:C:230:ILE:O	2.16	0.45
1:E:298:ASN:HD22	1:E:298:ASN:H	1.64	0.45
1:E:132:GLY:HA3	1:E:152:TRP:HB3	1.99	0.45
1:A:78:TRP:NE1	1:A:110:GLY:O	2.50	0.45
1:C:110:GLY:HA3	1:C:260:PHE:CZ	2.52	0.45
1:E:301:PRO:HD3	1:E:310:TYR:CZ	2.51	0.45
1:E:40:GLU:HB2	1:E:289:VAL:HB	1.99	0.44
1:A:46:ILE:CD1	1:A:304:ILE:HG23	2.44	0.44
2:D:25:HIS:CD2	2:D:33:GLY:O	2.70	0.44
2:F:29:SER:OG	2:F:143:LYS:HE2	2.18	0.44
1:A:23:GLU:CD	1:A:323:ARG:HH22	2.21	0.44
1:E:118:MET:HE2	1:E:257:ALA:CB	2.47	0.44
2:D:38:ARG:HG2	2:D:38:ARG:HH11	1.83	0.44
1:E:279:CYS:SG	1:E:291:ARG:NH2	2.91	0.44
1:A:94:PRO:HG3	1:A:226:GLN:HB2	2.00	0.44
1:E:297:GLN:HG2	1:E:308:PRO:HD2	1.98	0.44
1:A:165:LYS:HA	1:A:245:VAL:O	2.18	0.44
1:A:59:ILE:O	1:A:63:ILE:HG13	2.16	0.44
1:A:310:TYR:CD2	2:B:89:LEU:HD13	2.53	0.44
1:C:71:LEU:HD12	1:C:72:LEU:HD13	1.99	0.44
1:C:83:GLU:O	1:C:271:LYS:HA	2.18	0.44
1:A:201:TYR:CD2	1:A:203:ARG:HG3	2.52	0.44
1:A:121:LYS:HE3	1:A:255:TRP:CZ2	2.53	0.43
1:A:186:LEU:HD22	1:A:227:ARG:HB2	1.99	0.43
1:C:200:LYS:O	1:C:214:SER:HB2	2.19	0.43
1:E:118:MET:HE1	1:E:178:TYR:CB	2.48	0.43
1:E:175:PRO:HD2	1:E:260:PHE:O	2.18	0.43
1:A:155:LYS:NZ	1:A:158:SER:O	2.43	0.43
1:C:93:TYR:HD2	1:C:134:THR:HG21	1.83	0.43
1:C:170:ASN:HB3	4:C:405:HOH:O	2.17	0.43
1:E:292:THR:OG1	1:E:294:LYS:HG3	2.18	0.43
1:E:105:ALA:O	1:E:108:GLY:O	2.36	0.43
1:E:124:TRP:CD1	1:E:153:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ASP:HB3	1:A:233:TYR:CE2	2.54	0.43
1:C:186:LEU:HA	1:C:218:ALA:O	2.18	0.43
1:C:63:ILE:HA	1:C:63:ILE:HD12	1.90	0.43
1:C:4:LYS:CE	2:D:25:HIS:HE1	2.32	0.43
2:D:2:ILE:HG21	2:D:2:ILE:HD13	1.77	0.43
1:A:52:LEU:HD13	1:A:76:GLN:HG3	2.00	0.43
1:A:220:ARG:HB3	1:A:229:ARG:NH1	2.34	0.43
1:C:102:GLU:OE2	2:F:75:ARG:N	2.41	0.43
1:E:114:GLU:HB2	1:E:259:LYS:HB2	1.99	0.43
1:A:2:GLY:HA3	2:B:139:GLU:OE1	2.19	0.43
1:C:220:ARG:NE	4:C:421:HOH:O	2.52	0.43
1:A:93:TYR:CE1	1:A:230:ILE:HG13	2.54	0.42
1:A:23:GLU:OE2	1:A:323:ARG:NH2	2.49	0.42
2:B:20:GLY:HA3	2:B:36:ALA:HB1	1.99	0.42
1:A:290:LEU:HD21	1:A:299:VAL:HG21	2.02	0.42
2:B:167:LYS:O	2:B:171:GLN:HG2	2.20	0.42
1:A:64:LEU:O	1:A:147:TYR:HB3	2.19	0.42
1:C:135:ASN:N	1:C:135:ASN:OD1	2.46	0.42
1:A:187:ASP:CB	1:A:190:VAL:H	2.32	0.42
2:B:2:ILE:HG23	2:B:3:PHE:CD1	2.54	0.42
1:A:8:GLY:HA3	2:B:14:TRP:CH2	2.55	0.42
1:A:53:ASP:HB2	1:A:276:ILE:HD12	2.02	0.42
2:B:170:ARG:NH2	4:B:210:HOH:O	2.53	0.42
2:F:19:ASP:OD1	2:F:19:ASP:N	2.53	0.42
2:F:30:GLN:HE22	2:F:146:ASN:H	1.67	0.42
2:B:141:TRP:CE2	2:B:170:ARG:HG3	2.55	0.42
1:C:151:VAL:HG23	1:C:255:TRP:HB2	2.02	0.42
1:C:75:ASP:OD1	1:C:75:ASP:N	2.53	0.42
1:C:97:LEU:HA	1:C:232:TYR:HB2	2.01	0.42
1:E:182:VAL:HG21	1:E:213:LYS:HB3	2.02	0.42
2:B:94:TYR:OH	2:B:98:LEU:HD22	2.20	0.41
1:E:285:THR:CG2	1:E:300:SER:HB3	2.49	0.41
2:B:158:ASP:OD1	2:B:160:PRO:HD2	2.19	0.41
1:A:11:ALA:HB2	2:B:13:GLY:HA3	2.01	0.41
1:C:301:PRO:HD3	1:C:310:TYR:CZ	2.56	0.41
2:D:167:LYS:HA	2:D:170:ARG:NE	2.33	0.41
2:B:99:LEU:HD13	2:D:98:LEU:HD21	2.02	0.41
4:C:445:HOH:O	1:E:229:ARG:HD2	2.20	0.41
1:A:184:HIS:HB3	1:A:216:GLU:O	2.19	0.41
2:B:104:ASN:O	2:B:108:LEU:HG	2.21	0.41
2:F:54:SER:O	2:F:58:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:LEU:CD1	1:C:72:LEU:HD13	2.50	0.41
1:E:201:TYR:CD1	1:E:248:ASN:HB2	2.56	0.41
1:A:263:THR:HG23	1:A:265:LYS:O	2.21	0.41
2:B:20:GLY:HA3	2:B:36:ALA:CB	2.50	0.41
1:E:112:ARG:HB3	1:E:261:VAL:HG12	2.02	0.41
1:E:296:PHE:HZ	2:F:59:MET:HG3	1.86	0.41
1:A:111:GLU:O	1:A:112:ARG:HB3	2.20	0.41
1:A:152:TRP:CD1	1:A:152:TRP:C	2.94	0.41
1:C:156:THR:C	1:C:159:ALA:HB2	2.38	0.41
2:F:9:PHE:O	2:F:135:ASN:HA	2.21	0.41
1:A:186:LEU:CD2	1:A:227:ARG:HB2	2.50	0.41
2:B:27:GLU:HG3	2:B:32:SER:HB3	2.02	0.41
1:C:4:LYS:HG2	2:D:27:GLU:CB	2.49	0.41
1:E:201:TYR:CE1	1:E:248:ASN:HB2	2.56	0.41
1:A:201:TYR:HD2	1:A:203:ARG:HG3	1.86	0.41
1:A:237:LEU:HD12	1:A:241:GLU:HB3	2.02	0.41
1:C:167:THR:HA	1:C:243:LEU:O	2.20	0.41
1:A:78:TRP:CE2	1:A:110:GLY:O	2.73	0.41
1:A:21:LEU:HB2	2:B:105:GLU:OE2	2.20	0.41
1:C:218:ALA:O	1:C:220:ARG:NH1	2.51	0.41
1:E:118:MET:HE3	1:E:118:MET:HB3	1.89	0.41
1:E:8:GLY:HA3	2:F:14:TRP:CH2	2.55	0.40
1:A:63:ILE:H	1:A:63:ILE:HG13	1.57	0.40
1:C:170:ASN:ND2	1:C:176:ILE:HD12	2.36	0.40
1:E:73:LEU:HD11	1:E:115:ARG:CZ	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	328/333 (98%)	323 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	321/333 (96%)	315 (98%)	6 (2%)	0	100	100
1	E	321/333 (96%)	312 (97%)	9 (3%)	0	100	100
2	B	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
2	D	171/180 (95%)	168 (98%)	3 (2%)	0	100	100
2	F	170/180 (94%)	165 (97%)	5 (3%)	0	100	100
All	All	1482/1539 (96%)	1452 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	290/292 (99%)	284 (98%)	6 (2%)	59	70
1	C	285/292 (98%)	280 (98%)	5 (2%)	64	75
1	E	286/292 (98%)	281 (98%)	5 (2%)	66	77
2	B	147/153 (96%)	143 (97%)	4 (3%)	50	60
2	D	147/153 (96%)	145 (99%)	2 (1%)	71	82
2	F	146/153 (95%)	145 (99%)	1 (1%)	87	93
All	All	1301/1335 (98%)	1278 (98%)	23 (2%)	64	75

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

Mol	Chain	Res	Type
1	A	24	LYS
1	A	73	LEU
1	A	112	ARG
1	A	161	TYR
1	A	225	ASP
1	A	264	ASN
2	B	22	TYR
2	B	67	ASP

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Mol	Chain	Res	Type
2	B	163	GLN
2	B	171	GLN
1	C	75	ASP
1	C	157	ASP
1	C	225	ASP
1	C	291	ARG
1	C	322	LEU
2	D	22	TYR
2	D	118	LEU
1	E	47	MET
1	E	225	ASP
1	E	291	ARG
1	E	295	THR
1	E	298	ASN
2	F	22	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	297	GLN
2	B	30	GLN
1	C	278	ASN
2	D	25	HIS
1	E	244	ASN
1	E	298	ASN
2	F	30	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	NAG	A	401	1	14,14,15	0.59	0	15,19,21	1.10	1 (6%)
3	NAG	A	402	1	14,14,15	0.64	0	15,19,21	1.81	4 (26%)
3	NAG	E	401	1	14,14,15	0.48	0	15,19,21	1.53	3 (20%)
3	NAG	E	402	1	14,14,15	0.73	0	15,19,21	1.53	3 (20%)

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	NAG	A	401	1	-	0/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	1/6/23/26	0/1/1/1
3	NAG	E	402	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	NAG	C6-C5-C4	-3.87	103.94	113.00
3	E	402	NAG	C6-C5-C4	-3.71	104.33	113.00
3	E	402	NAG	O3-C3-C2	-2.94	103.09	109.39
3	E	401	NAG	C1-C2-N2	-2.75	105.79	110.49
3	A	401	NAG	O6-C6-C5	-2.26	103.73	111.34
3	A	402	NAG	C2-N2-C7	-2.17	119.78	122.94
3	E	402	NAG	C1-O5-C5	2.70	115.89	112.17
3	E	401	NAG	C1-O5-C5	2.74	115.94	112.17
3	A	402	NAG	C1-O5-C5	2.76	115.97	112.17
3	E	401	NAG	C2-N2-C7	3.36	127.84	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	NAG	C1-C2-N2	4.25	117.74	110.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	401	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	330/333 (99%)	0.22	8 (2%)	59	60	30, 49, 66, 86	0
1	C	325/333 (97%)	0.16	12 (3%)	42	42	31, 43, 58, 87	0
1	E	325/333 (97%)	0.11	6 (1%)	69	69	31, 43, 56, 80	0
2	B	173/180 (96%)	0.41	4 (2%)	61	61	31, 40, 60, 77	0
2	D	173/180 (96%)	0.55	11 (6%)	20	21	31, 42, 61, 87	0
2	F	172/180 (95%)	0.33	9 (5%)	28	29	32, 42, 57, 85	0
All	All	1498/1539 (97%)	0.26	50 (3%)	47	47	30, 43, 61, 87	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	173	ILE	9.5
1	C	158	SER	7.6
2	D	1	GLY	7.0
2	B	1	GLY	6.3
2	F	1	GLY	6.1
1	C	329	ALA	5.0
2	B	173	ILE	4.9
2	D	171	GLN	4.4
1	A	154	VAL	4.3
2	F	171	GLN	4.3
1	A	131	ARG	4.3
2	D	168	LEU	4.1
1	C	157	ASP	3.8
1	E	159	ALA	3.7
1	E	1	PRO	3.7
1	E	108	GLY	3.5
1	A	329	ALA	3.3
2	D	164	LYS	3.3
2	F	2	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	158	SER	3.2
2	D	163	GLN	3.1
2	D	170	ARG	3.1
2	D	172	GLY	2.9
2	B	2	ILE	2.8
2	F	141	TRP	2.7
1	A	13	ASN	2.7
1	C	86	ASN	2.6
1	A	264	ASN	2.6
1	A	46	ILE	2.5
2	F	168	LEU	2.5
1	C	4	LYS	2.5
2	F	38	ARG	2.5
2	D	2	ILE	2.5
1	C	190	VAL	2.5
1	C	47	MET	2.4
2	F	172	GLY	2.4
1	A	48	ASN	2.3
1	C	38	GLN	2.3
2	B	18	ILE	2.3
2	F	134	GLY	2.3
1	C	193	ASN	2.3
2	D	4	GLY	2.3
2	D	10	ILE	2.3
2	F	113	ALA	2.2
1	C	194	LEU	2.2
1	A	265	LYS	2.2
1	E	279	CYS	2.1
1	E	74	GLY	2.1
1	C	160	THR	2.1
1	C	225	ASP	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 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, 95th 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
3	NAG	E	402	14/15	0.83	0.19	0.71	59,68,74,74	0
3	NAG	A	402	14/15	0.83	0.12	-0.53	65,68,73,76	0
3	NAG	A	401	14/15	0.76	0.20	-	56,75,78,83	0
3	NAG	E	401	14/15	0.78	0.37	-	80,87,91,95	0

6.5 Other polymers (i)

There are no such residues in this entry.