Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:10 PM GMT

PDB ID	:	4NYL
Title	:	Crystal structure of adalimumab FAB fragment
Authors	:	Fan, L.J.; Lv, L.L.; Zhang, Q.J.; Chen, C.L.
Deposited on	:	2013-12-10
Resolution	:	2.80 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:

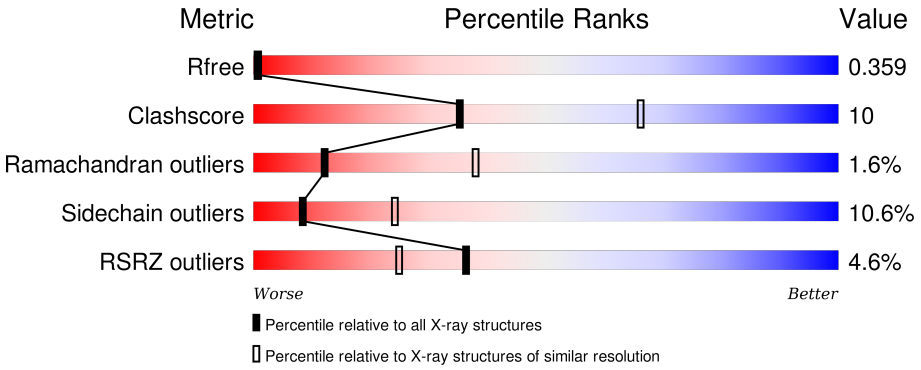
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	B	214	3% 41% 11% • 45%
1	D	214	77% 19% • •
1	F	214	8% 46% 9% • 42%
1	L	214	2% 78% 19% • •
2	A	230	12% 68% 16% • 13%

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Mol	Chain	Length	Quality of chain
2	C	230	73% 15% 7%
2	E	230	3% 54% 14% 30%
2	H	230	66% 22% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10495 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 Adalimumab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1546	966	262	313	5			
1	B	117	Total	C	N	O	S	0	0	0
			829	518	144	164	3			
1	D	211	Total	C	N	O	S	0	0	0
			1557	972	261	319	5			
1	F	124	Total	C	N	O	S	0	0	0
			876	543	149	181	3			

- Molecule 2 is a protein called Adalimumab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	0	0
			1564	991	263	304	6			
2	A	199	Total	C	N	O	S	0	0	0
			1405	879	239	281	6			
2	C	213	Total	C	N	O	S	0	0	0
			1561	987	263	305	6			
2	E	162	Total	C	N	O	S	0	1	0
			1155	723	200	228	4			

- Molecule 3 is water.

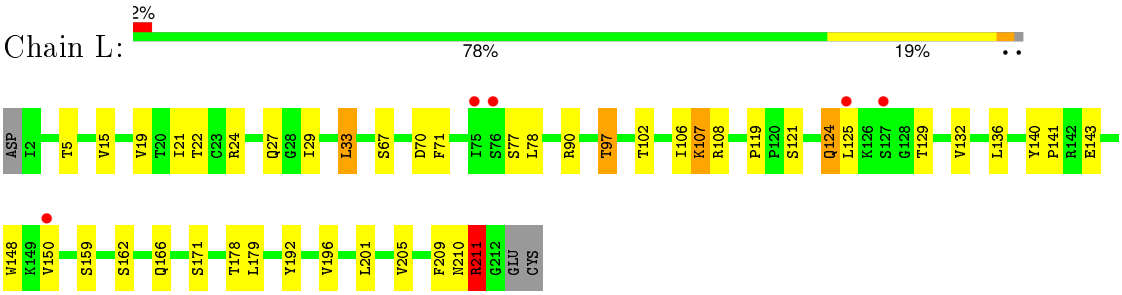
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		
3	C	1	Total	O	0	0
			1	1		

3 Residue-property plots

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.

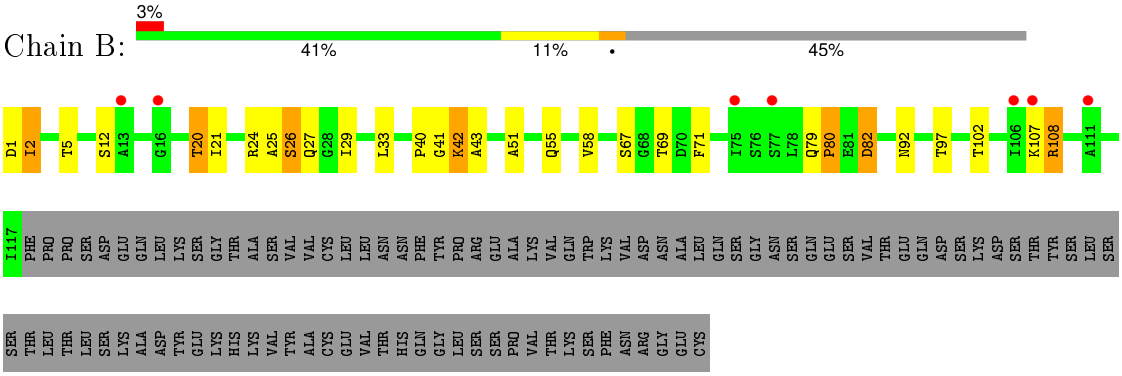
- Molecule 1: Adalimumab Light Chain

Chain L:



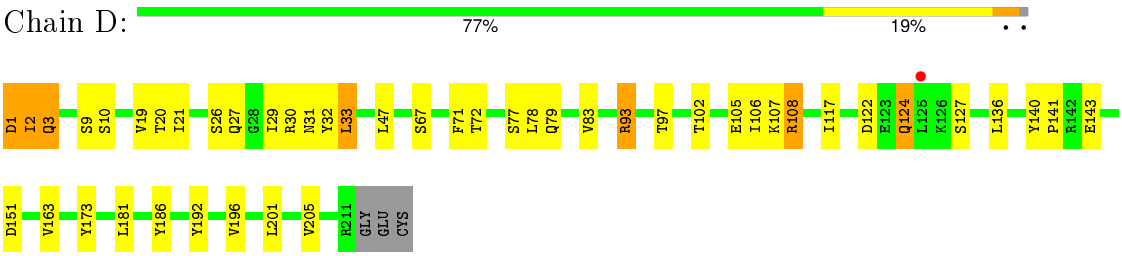
- Molecule 1: Adalimumab Light Chain

Chain B:



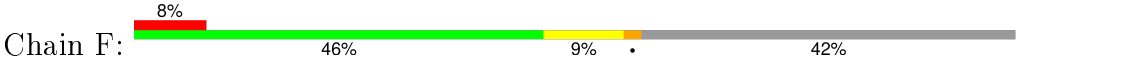
- Molecule 1: Adalimumab Light Chain

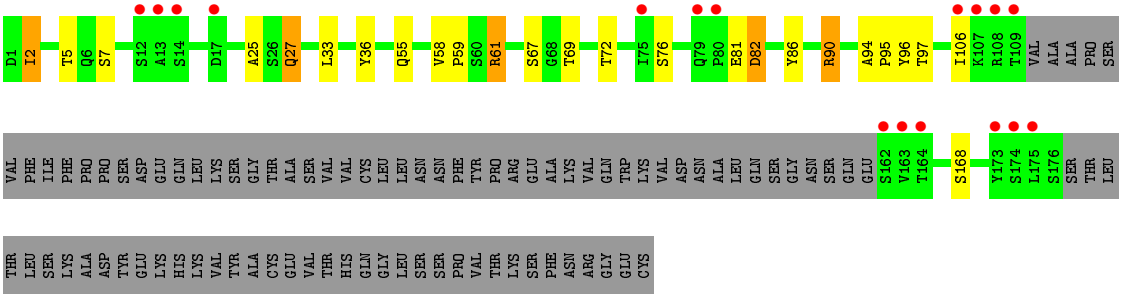
Chain D:



- Molecule 1: Adalimumab Light Chain

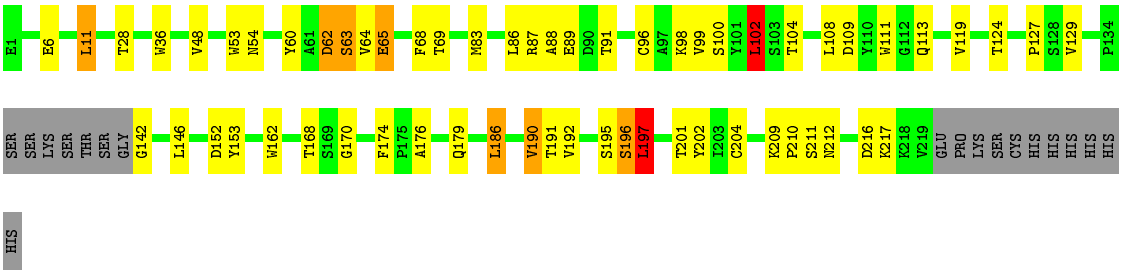
Chain F:





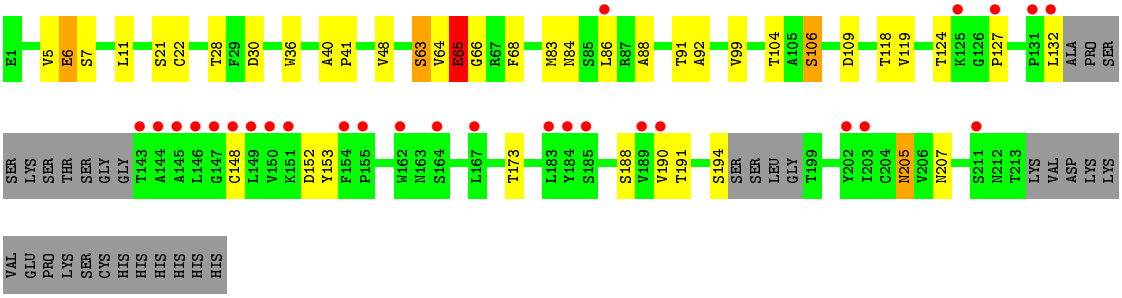
• Molecule 2: Adalimumab Heavy Chain

Chain H:



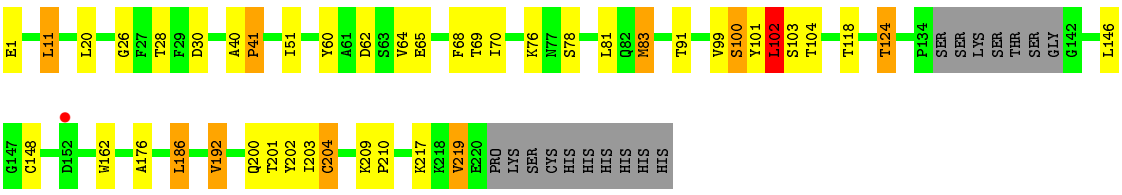
• Molecule 2: Adalimumab Heavy Chain

Chain A:



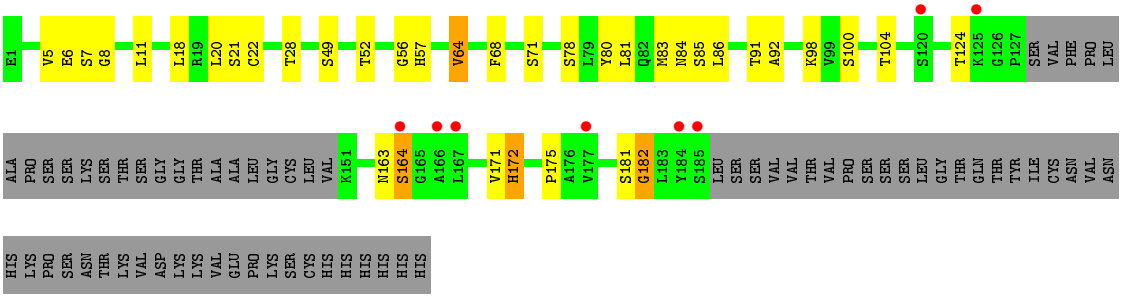
• Molecule 2: Adalimumab Heavy Chain

Chain C:



• Molecule 2: Adalimumab Heavy Chain

Chain E:


E1 V5 E6 S7 G8 L11 L18 R19 L20 S21 C22 T28 S49 T52 G56 H57 V64 F68 S71 S78 L79 Y80 L81 Q82 M83 N84 S85 L86 T91 A92 K98 V99 S100 T104 S120 T124 K125 G126 P127 SER VAL PHE PRO LEU
ALA PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA LEU GLY CYS LEU VAL K151 N163 S164 G165 A166 L167 V171 H172 P175 A176 V177 S181 G182 L183 Y184 S185 LEU SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN
HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER CYS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.42Å 47.05Å 168.51Å 90.00° 101.33° 90.00°	Depositor
Resolution (Å)	42.03 – 2.80 40.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.1 (42.03-2.80) 87.1 (40.11-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.275 , 0.358 0.273 , 0.359	Depositor DCC
R_{free} test set	2249 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 44308 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	10495	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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	B	0.53	0/848	0.73	0/1161
1	D	0.55	0/1591	0.74	1/2177 (0.0%)
1	F	0.49	0/892	0.69	0/1221
1	L	0.53	0/1580	0.75	0/2162
2	A	0.50	0/1438	0.68	0/1974
2	C	0.57	0/1599	0.77	3/2189 (0.1%)
2	E	0.54	0/1186	0.72	0/1623
2	H	0.62	1/1602 (0.1%)	0.80	0/2189
All	All	0.55	1/10736 (0.0%)	0.74	4/14696 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	142	GLY	N-CA	-5.14	1.38	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	103	SER	N-CA-C	-5.74	95.49	111.00
1	D	93	ARG	NE-CZ-NH1	5.73	123.17	120.30
2	C	102	LEU	CA-CB-CG	5.54	128.05	115.30
2	C	30	ASP	CB-CG-OD2	5.00	122.80	118.30

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	B	829	0	747	20	0
1	D	1557	0	1433	25	0
1	F	876	0	773	15	0
1	L	1546	0	1422	29	0
2	A	1405	0	1243	19	0
2	C	1561	0	1472	27	0
2	E	1155	0	1019	20	0
2	H	1564	0	1489	42	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	10495	0	9598	197	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 10.

All (197) 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)
2:H:196:SER:OG	2:H:197:LEU:HD23	1.51	1.10
2:A:40:ALA:HB1	2:A:41:PRO:HD2	1.42	1.01
1:L:107:LYS:CB	1:L:108:ARG:HA	1.92	1.00
2:H:88:ALA:O	2:H:91:THR:HG23	1.66	0.94
2:H:197:LEU:HD23	2:H:197:LEU:N	1.87	0.88
2:H:64:VAL:HG11	2:H:68:PHE:HB2	1.55	0.88
1:L:107:LYS:CB	1:L:108:ARG:CA	2.54	0.84
1:B:20:THR:CG2	1:B:20:THR:O	2.25	0.84
1:F:81:GLU:C	1:F:82:ASP:OD1	2.18	0.82
2:H:88:ALA:O	2:H:91:THR:CG2	2.28	0.81
2:A:64:VAL:O	2:A:65:GLU:C	2.21	0.78
1:B:20:THR:HG22	1:B:20:THR:O	1.88	0.73
2:A:64:VAL:HG11	2:A:68:PHE:HB2	1.70	0.73
2:H:196:SER:O	2:H:197:LEU:HB2	1.89	0.72
1:D:107:LYS:O	1:D:140:TYR:CZ	2.43	0.72
1:L:106:ILE:CG2	1:L:171:SER:HB3	2.19	0.72
1:D:1:ASP:O	1:D:2:ILE:C	2.27	0.72
2:C:91:THR:HG23	2:C:118:THR:HA	1.72	0.71
2:H:197:LEU:CD2	2:H:197:LEU:N	2.54	0.69
2:H:209:LYS:O	2:H:212:ASN:N	2.26	0.69
1:F:81:GLU:O	1:F:82:ASP:OD1	2.10	0.69
1:L:210:ASN:O	1:L:211:ARG:CG	2.41	0.68
2:H:91:THR:HG22	2:H:119:VAL:H	1.57	0.68
2:A:64:VAL:O	2:A:66:GLY:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:106:ILE:HG21	1:L:171:SER:HB3	1.76	0.67
2:H:89:GLU:N	2:H:89:GLU:OE1	2.26	0.67
2:A:91:THR:HG23	2:A:118:THR:HA	1.76	0.66
2:E:64:VAL:HG21	2:E:68:PHE:HB2	1.76	0.66
2:H:11:LEU:HD12	2:H:124:THR:HG22	1.78	0.66
2:C:102:LEU:HD12	2:C:102:LEU:O	1.96	0.65
1:L:210:ASN:O	1:L:211:ARG:CB	2.43	0.65
2:H:209:LYS:O	2:H:210:PRO:C	2.35	0.65
2:C:81:LEU:HD23	2:C:83:MET:HE3	1.79	0.64
2:H:152:ASP:OD1	2:H:179:GLN:NE2	2.32	0.62
1:D:30:ARG:HG2	1:D:31:ASN:N	2.16	0.61
1:L:106:ILE:HG22	1:L:166:GLN:NE2	2.17	0.60
1:D:1:ASP:O	1:D:3:GLN:N	2.35	0.60
2:H:196:SER:OG	2:H:197:LEU:CD2	2.39	0.59
1:B:107:LYS:O	1:B:108:ARG:HB3	2.02	0.59
2:H:209:LYS:O	2:H:211:SER:N	2.36	0.58
1:L:106:ILE:HG21	1:L:171:SER:CB	2.34	0.58
2:A:40:ALA:HB1	2:A:41:PRO:CD	2.28	0.58
2:C:1:GLU:O	2:C:26:GLY:HA3	2.03	0.58
1:D:136:LEU:HD21	1:D:196:VAL:HG13	1.85	0.58
2:A:5:VAL:O	2:A:22:CYS:HA	2.04	0.57
2:H:196:SER:OG	2:H:197:LEU:N	2.35	0.56
1:L:136:LEU:HD21	1:L:196:VAL:HG13	1.86	0.56
2:C:64:VAL:CG1	2:C:68:PHE:CG	2.89	0.56
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.88	0.56
2:H:36:TRP:O	2:H:48:VAL:HB	2.06	0.56
2:H:64:VAL:HG12	2:H:65:GLU:N	2.20	0.56
2:C:100:SER:HB3	2:C:101:TYR:CD2	2.41	0.55
2:C:64:VAL:HG11	2:C:68:PHE:CD2	2.42	0.55
1:L:201:LEU:HD13	1:L:205:VAL:HG23	1.89	0.55
2:H:195:SER:C	2:H:196:SER:O	2.44	0.55
2:C:219:VAL:O	2:C:219:VAL:CG2	2.54	0.55
2:H:102:LEU:HD13	2:H:102:LEU:C	2.27	0.55
2:E:64:VAL:HG21	2:E:68:PHE:CB	2.37	0.54
2:H:162:TRP:CH2	2:H:204:CYS:HB3	2.43	0.54
2:A:64:VAL:HG11	2:A:68:PHE:CB	2.38	0.54
1:B:20:THR:HG23	1:B:20:THR:O	2.04	0.54
2:C:203:ILE:HG23	2:C:217:LYS:O	2.08	0.53
2:E:5:VAL:O	2:E:22:CYS:HA	2.08	0.53
1:B:21:ILE:HD13	1:B:102:THR:HG21	1.91	0.53
1:F:2:ILE:HG21	1:F:90:ARG:CZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:ALA:HA	1:F:95:PRO:C	2.29	0.53
2:C:11:LEU:HD13	2:C:124:THR:HG22	1.90	0.52
2:H:62:ASP:O	2:H:63:SER:HB2	2.09	0.52
2:H:192:VAL:HG11	2:H:202:TYR:CE2	2.44	0.52
2:C:162:TRP:CH2	2:C:204:CYS:HB3	2.45	0.52
1:B:40:PRO:O	1:B:40:PRO:CG	2.56	0.52
1:D:77:SER:O	1:D:79:GLN:OE1	2.27	0.52
1:L:24:ARG:CD	1:L:70:ASP:OD1	2.58	0.51
2:E:56:GLY:O	2:E:57[A]:HIS:CG	2.63	0.51
1:B:40:PRO:HG2	1:B:40:PRO:O	2.10	0.51
1:L:27:GLN:O	1:L:29:ILE:HG23	2.10	0.51
2:E:18:LEU:CD2	2:E:20:LEU:HD23	2.41	0.51
2:A:83:MET:HB3	2:A:86:LEU:HD21	1.93	0.50
2:A:173:THR:HA	2:A:188:SER:HA	1.92	0.50
2:C:1:GLU:O	2:C:26:GLY:CA	2.60	0.50
1:F:82:ASP:N	1:F:82:ASP:OD1	2.45	0.50
1:L:90:ARG:CD	1:L:97:THR:HG23	2.42	0.50
1:B:102:THR:HG23	1:B:102:THR:O	2.11	0.50
1:L:15:VAL:HA	1:L:78:LEU:O	2.12	0.50
1:B:92:ASN:N	1:B:92:ASN:OD1	2.45	0.49
2:H:6:GLU:HG3	2:H:96:CYS:SG	2.51	0.49
1:D:107:LYS:O	1:D:140:TYR:CE2	2.65	0.49
1:D:136:LEU:HD21	1:D:196:VAL:CG1	2.43	0.49
2:C:40:ALA:O	2:C:41:PRO:C	2.50	0.49
2:E:6:GLU:HA	2:E:21:SER:O	2.12	0.49
1:D:1:ASP:O	1:D:3:GLN:CB	2.61	0.49
2:C:64:VAL:HG12	2:C:68:PHE:HB2	1.95	0.49
2:E:83:MET:HB3	2:E:86:LEU:HD21	1.94	0.49
1:D:83:VAL:HG13	1:D:83:VAL:O	2.13	0.48
2:H:195:SER:O	2:H:196:SER:O	2.32	0.48
2:E:163:ASN:O	2:E:164:SER:CB	2.61	0.48
1:D:30:ARG:HG2	1:D:31:ASN:H	1.75	0.48
2:E:8:GLY:O	2:E:18:LEU:HD21	2.12	0.48
2:H:108:LEU:HD12	2:H:111:TRP:CZ2	2.49	0.48
1:D:27:GLN:O	1:D:29:ILE:HG23	2.12	0.48
2:C:219:VAL:O	2:C:219:VAL:HG23	2.12	0.48
2:H:62:ASP:O	2:H:63:SER:CB	2.61	0.48
2:A:127:PRO:HB3	2:A:153:TYR:HB3	1.94	0.48
2:E:52:THR:CG2	2:E:57[B]:HIS:HB2	2.44	0.48
1:B:27:GLN:O	1:B:29:ILE:HG23	2.12	0.48
2:C:64:VAL:CG1	2:C:68:PHE:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:O	1:B:108:ARG:CB	2.62	0.48
1:L:210:ASN:O	1:L:211:ARG:HB2	2.13	0.48
2:H:174:PHE:O	2:H:186:LEU:HD22	2.14	0.48
2:E:64:VAL:O	2:E:64:VAL:HG22	2.13	0.47
2:E:52:THR:HG23	2:E:57[B]:HIS:HB2	1.95	0.47
1:L:19:VAL:HG21	1:L:78:LEU:HD22	1.96	0.47
2:H:196:SER:O	2:H:197:LEU:CB	2.51	0.47
1:L:148:TRP:CE3	1:L:179:LEU:HD22	2.49	0.47
1:B:40:PRO:HA	1:B:41:GLY:HA2	1.58	0.47
2:E:18:LEU:HD21	2:E:20:LEU:HD23	1.97	0.47
1:D:105:GLU:OE1	1:D:173:TYR:OH	2.27	0.47
1:L:107:LYS:CB	1:L:108:ARG:CB	2.92	0.47
1:D:201:LEU:HD13	1:D:205:VAL:HG23	1.95	0.47
1:L:90:ARG:HD3	1:L:97:THR:HG23	1.96	0.47
2:H:91:THR:HG22	2:H:119:VAL:N	2.29	0.46
2:H:129:VAL:O	2:H:217:LYS:HE3	2.15	0.46
1:B:33:LEU:HD22	1:B:71:PHE:CG	2.51	0.46
1:D:124:GLN:O	1:D:127:SER:CB	2.64	0.46
1:L:107:LYS:CB	1:L:108:ARG:HB3	2.45	0.46
2:C:20:LEU:HD11	2:C:83:MET:HE1	1.97	0.46
2:C:192:VAL:HG11	2:C:202:TYR:CE1	2.50	0.46
2:H:196:SER:O	2:H:197:LEU:O	2.33	0.46
2:H:53:TRP:CZ2	2:H:54:ASN:ND2	2.83	0.46
1:B:1:ASP:O	1:B:2:ILE:HG22	2.16	0.46
1:D:141:PRO:HB2	1:D:143:GLU:OE1	2.16	0.45
2:E:20:LEU:HD12	2:E:81:LEU:HD23	1.98	0.45
2:C:146:LEU:HD12	2:C:146:LEU:C	2.37	0.45
1:L:121:SER:O	1:L:125:LEU:HD12	2.17	0.45
2:A:36:TRP:O	2:A:48:VAL:HB	2.16	0.45
2:E:64:VAL:HG21	2:E:68:PHE:CG	2.52	0.44
1:F:94:ALA:HB2	1:F:96:TYR:CE1	2.52	0.44
2:C:176:ALA:HA	2:C:186:LEU:HD23	1.98	0.44
1:B:55:GLN:O	1:B:58:VAL:HB	2.17	0.44
2:A:6:GLU:HA	2:A:21:SER:O	2.16	0.44
1:D:29:ILE:O	1:D:32:TYR:HD1	2.00	0.44
2:H:170:GLY:O	2:H:190:VAL:HA	2.17	0.44
1:B:25:ALA:O	1:B:69:THR:HB	2.18	0.44
2:A:88:ALA:HA	2:A:119:VAL:HB	1.99	0.44
1:F:25:ALA:O	1:F:69:THR:HB	2.17	0.44
1:B:33:LEU:HD22	1:B:71:PHE:CD1	2.52	0.44
1:B:42:LYS:HG3	1:B:43:ALA:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:ASP:O	1:D:3:GLN:HB2	2.18	0.44
1:L:140:TYR:CG	1:L:141:PRO:HA	2.53	0.43
2:H:176:ALA:HA	2:H:186:LEU:HD23	2.00	0.43
1:D:107:LYS:O	1:D:108:ARG:O	2.36	0.43
2:C:64:VAL:O	2:C:65:GLU:C	2.56	0.43
1:D:33:LEU:HD22	1:D:71:PHE:CD2	2.53	0.43
2:C:81:LEU:CD2	2:C:83:MET:HE3	2.48	0.43
1:F:90:ARG:NH1	1:F:95:PRO:O	2.52	0.43
1:L:119:PRO:HB3	1:L:209:PHE:CE2	2.53	0.43
2:C:209:LYS:O	2:C:210:PRO:C	2.57	0.43
2:C:101:TYR:O	2:C:102:LEU:HG	2.18	0.42
1:F:2:ILE:HG23	1:F:2:ILE:O	2.18	0.42
1:L:150:VAL:HG13	1:L:192:TYR:CE2	2.54	0.42
2:E:91:THR:O	2:E:92:ALA:HB2	2.19	0.42
2:H:83:MET:HB3	2:H:86:LEU:HD21	2.01	0.42
1:D:30:ARG:CG	1:D:31:ASN:N	2.75	0.42
1:D:186:TYR:HA	1:D:192:TYR:OH	2.19	0.42
1:F:36:TYR:O	1:F:86:TYR:HA	2.19	0.42
2:E:84:ASN:O	2:E:85:SER:C	2.58	0.42
1:F:2:ILE:HG13	1:F:27:GLN:HG3	2.01	0.42
1:F:59:PRO:HB2	1:F:61:ARG:HD2	2.01	0.42
2:C:60:TYR:OH	2:C:69:THR:HA	2.19	0.42
1:L:159:SER:HA	1:L:178:THR:O	2.20	0.42
1:L:132:VAL:HB	1:L:179:LEU:HB3	2.00	0.42
1:F:2:ILE:CG1	1:F:27:GLN:HG3	2.50	0.42
1:D:21:ILE:HG12	1:D:102:THR:HG21	2.02	0.42
2:A:40:ALA:CB	2:A:41:PRO:CD	2.95	0.41
2:H:98:LYS:HG2	2:H:99:VAL:N	2.33	0.41
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.55	0.41
2:H:68:PHE:CE2	2:H:83:MET:HG2	2.56	0.41
2:E:71:SER:O	2:E:80:TYR:N	2.49	0.41
2:H:217:LYS:HD3	2:H:217:LYS:O	2.21	0.41
1:D:3:GLN:HB3	1:D:26:SER:HB3	2.02	0.41
1:B:2:ILE:HA	1:B:26:SER:OG	2.19	0.41
2:E:181:SER:N	2:E:182:GLY:HA2	2.36	0.41
1:L:136:LEU:HD21	1:L:196:VAL:CG1	2.50	0.41
2:H:60:TYR:OH	2:H:69:THR:HA	2.21	0.41
2:A:91:THR:O	2:A:92:ALA:HB2	2.21	0.41
1:F:61:ARG:HB3	1:F:76:SER:OG	2.21	0.41
2:A:205:ASN:N	2:A:205:ASN:OD1	2.54	0.41
1:F:55:GLN:O	1:F:58:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:VAL:CG1	2:C:68:PHE:CD2	3.04	0.41
2:E:171:VAL:O	2:E:172:HIS:ND1	2.54	0.40
2:C:51:ILE:HG22	2:C:70:ILE:HD11	2.03	0.40
1:L:21:ILE:HG12	1:L:102:THR:HG21	2.03	0.40
2:A:99:VAL:HG13	2:A:106:SER:HB3	2.03	0.40
2:H:102:LEU:HD22	2:H:102:LEU:HA	1.85	0.40
1:B:79:GLN:CB	1:B:80:PRO:CD	2.99	0.40
1:D:19:VAL:HG21	1:D:78:LEU:HD22	2.04	0.40
2:A:190:VAL:HG12	2:A:191:THR:N	2.37	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	B	115/214 (54%)	97 (84%)	13 (11%)	5 (4%)	3 10
1	D	209/214 (98%)	183 (88%)	24 (12%)	2 (1%)	19 52
1	F	120/214 (56%)	108 (90%)	12 (10%)	0	100 100
1	L	209/214 (98%)	195 (93%)	10 (5%)	4 (2%)	10 32
2	A	193/230 (84%)	168 (87%)	22 (11%)	3 (2%)	12 38
2	C	209/230 (91%)	196 (94%)	12 (6%)	1 (0%)	34 69
2	E	159/230 (69%)	139 (87%)	17 (11%)	3 (2%)	10 32
2	H	208/230 (90%)	189 (91%)	14 (7%)	5 (2%)	7 25
All	All	1422/1776 (80%)	1275 (90%)	124 (9%)	23 (2%)	12 38

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	107	LYS

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Mol	Chain	Res	Type
1	L	124	GLN
1	L	211	ARG
2	H	102	LEU
2	H	196	SER
1	B	82	ASP
2	A	65	GLU
1	D	108	ARG
1	L	77	SER
2	H	63	SER
2	H	65	GLU
1	B	2	ILE
1	B	108	ARG
2	A	152	ASP
2	E	164	SER
1	B	80	PRO
1	D	2	ILE
2	E	175	PRO
2	E	182	GLY
1	B	51	ALA
2	H	197	LEU
2	A	63	SER
2	C	41	PRO

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	B	80/186 (43%)	71 (89%)	9 (11%)	7 22
1	D	165/186 (89%)	147 (89%)	18 (11%)	8 23
1	F	85/186 (46%)	72 (85%)	13 (15%)	3 10
1	L	162/186 (87%)	152 (94%)	10 (6%)	23 54
2	A	138/194 (71%)	121 (88%)	17 (12%)	6 18
2	C	165/194 (85%)	147 (89%)	18 (11%)	8 23
2	E	110/194 (57%)	99 (90%)	11 (10%)	9 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	166/194 (86%)	149 (90%)	17 (10%)	9 26
All	All	1071/1520 (70%)	958 (89%)	113 (11%)	8 24

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	22	THR
1	L	33	LEU
1	L	67	SER
1	L	97	THR
1	L	124	GLN
1	L	129	THR
1	L	143	GLU
1	L	162	SER
1	L	211	ARG
2	H	11	LEU
2	H	28	THR
2	H	62	ASP
2	H	87	ARG
2	H	100	SER
2	H	102	LEU
2	H	104	THR
2	H	109	ASP
2	H	113	GLN
2	H	146	LEU
2	H	168	THR
2	H	186	LEU
2	H	190	VAL
2	H	191	THR
2	H	197	LEU
2	H	201	THR
2	H	216	ASP
1	B	5	THR
1	B	12	SER
1	B	20	THR
1	B	24	ARG
1	B	26	SER
1	B	42	LYS
1	B	67	SER
1	B	82	ASP
1	B	97	THR

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Mol	Chain	Res	Type
2	A	6	GLU
2	A	7	SER
2	A	11	LEU
2	A	28	THR
2	A	30	ASP
2	A	63	SER
2	A	65	GLU
2	A	84	ASN
2	A	104	THR
2	A	106	SER
2	A	109	ASP
2	A	124	THR
2	A	132	LEU
2	A	148	CYS
2	A	194	SER
2	A	205	ASN
2	A	207	ASN
1	D	1	ASP
1	D	3	GLN
1	D	9	SER
1	D	10	SER
1	D	20	THR
1	D	33	LEU
1	D	47	LEU
1	D	67	SER
1	D	72	THR
1	D	93	ARG
1	D	97	THR
1	D	106	ILE
1	D	117	ILE
1	D	122	ASP
1	D	124	GLN
1	D	151	ASP
1	D	163	VAL
1	D	181	LEU
2	C	11	LEU
2	C	28	THR
2	C	62	ASP
2	C	76	LYS
2	C	78	SER
2	C	83	MET
2	C	99	VAL

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Mol	Chain	Res	Type
2	C	100	SER
2	C	102	LEU
2	C	104	THR
2	C	124	THR
2	C	148	CYS
2	C	186	LEU
2	C	192	VAL
2	C	200	GLN
2	C	201	THR
2	C	204	CYS
2	C	219	VAL
1	F	2	ILE
1	F	5	THR
1	F	7	SER
1	F	27	GLN
1	F	33	LEU
1	F	61	ARG
1	F	67	SER
1	F	72	THR
1	F	82	ASP
1	F	90	ARG
1	F	97	THR
1	F	106	ILE
1	F	168	SER
2	E	7	SER
2	E	11	LEU
2	E	28	THR
2	E	49	SER
2	E	64	VAL
2	E	78	SER
2	E	98	LYS
2	E	100	SER
2	E	104	THR
2	E	124	THR
2	E	172	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	79	GLN
1	L	137	ASN

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Mol	Chain	Res	Type
1	L	189	HIS
2	H	113	GLN
2	H	163	ASN
2	H	200	GLN
2	C	163	ASN
2	C	200	GLN
2	C	207	ASN
1	F	3	GLN
1	F	38	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	B	117/214 (54%)	0.20	7 (5%) 25 15	49, 83, 104, 140	0
1	D	211/214 (98%)	-0.20	1 (0%) 91 88	44, 63, 82, 93	0
1	F	124/214 (57%)	0.41	17 (13%) 4 2	54, 83, 103, 121	0
1	L	211/214 (98%)	-0.17	5 (2%) 62 50	46, 64, 85, 99	0
2	A	199/230 (86%)	0.35	27 (13%) 4 2	47, 75, 116, 126	0
2	C	213/230 (92%)	-0.26	1 (0%) 91 88	37, 64, 79, 98	0
2	E	162/230 (70%)	0.06	8 (4%) 33 22	45, 69, 122, 140	0
2	H	212/230 (92%)	-0.29	0 100 100	45, 61, 76, 101	0
All	All	1449/1776 (81%)	-0.03	66 (4%) 36 25	37, 66, 102, 140	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	ILE	7.1
2	A	150	VAL	5.6
2	E	166	ALA	5.5
1	F	174	SER	5.3
1	F	80	PRO	4.7
2	A	147	GLY	4.4
2	A	184	TYR	4.3
1	F	162	SER	4.3
2	A	125	LYS	4.1
2	E	177	VAL	4.1
1	F	164	THR	4.0
2	E	167	LEU	4.0
1	B	111	ALA	3.8
1	F	163	VAL	3.7
2	E	185	SER	3.6
2	A	185	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	75	ILE	3.5
2	A	145	ALA	3.4
2	A	190	VAL	3.4
1	F	14	SER	3.2
2	A	143	THR	3.1
2	A	148	CYS	3.1
1	F	106	ILE	3.1
2	A	154	PHE	3.0
2	A	149	LEU	3.0
1	B	13	ALA	3.0
2	A	183	LEU	2.9
2	E	164	SER	2.9
2	A	131	PRO	2.9
1	F	109	THR	2.9
2	E	120	SER	2.9
1	B	77	SER	2.8
2	A	162	TRP	2.8
2	A	164	SER	2.8
1	L	150	VAL	2.7
2	A	211	SER	2.6
1	F	13	ALA	2.5
1	D	125	LEU	2.5
1	F	75	ILE	2.5
2	A	202	TYR	2.5
1	B	107	LYS	2.5
1	B	16	GLY	2.5
2	A	155	PRO	2.4
1	F	17	ASP	2.4
1	F	175	LEU	2.4
2	A	203	ILE	2.4
1	L	125	LEU	2.4
1	F	108	ARG	2.4
1	F	173	TYR	2.4
2	A	144	ALA	2.4
1	L	75	ILE	2.4
2	C	152	ASP	2.3
2	A	189	VAL	2.3
2	A	151	LYS	2.3
1	F	79	GLN	2.3
2	A	86	LEU	2.3
2	A	132	LEU	2.3
2	E	184	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	125	LYS	2.2
2	A	127	PRO	2.2
1	L	127	SER	2.1
2	A	167	LEU	2.1
2	A	146	LEU	2.1
1	F	12	SER	2.1
1	F	107	LYS	2.0
1	L	76	SER	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.