Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 09:04 PM EDT

PDB ID	:	3I50
Title	:	Crystal structure of the West Nile Virus envelope glycoprotein in complex with the E53 antibody Fab
Authors	:	Nybakken, G.E.; Warren, J.T.; Chen, B.R.; Nelson, C.A.; Fremont, D.H.
Deposited on	:	2009-07-03
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

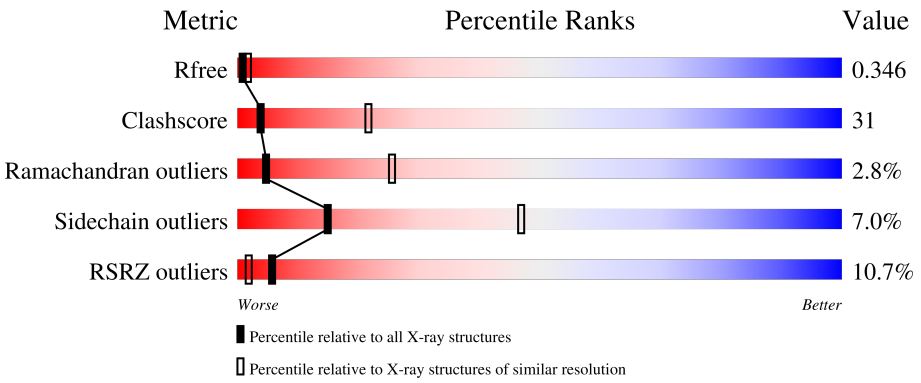
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	402	3%; 33%, 31%, •, 32%
2	L	207	14%; 49%, 46%, •
3	H	221	14%; 45%, 48%, •, •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5283 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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	273	2088	1312	359	399	18	0	0	0

- Molecule 2 is a protein called murine kappa light chain of E53 monoclonal antibody Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	207	1583	986	262	326	9	0	0	0

- Molecule 3 is a protein called murine heavy chain (IgG3) of E53 monoclonal antibody Fab.

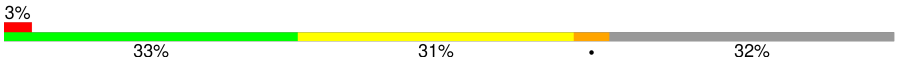
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	212	1612	1036	258	312	6	0	0	0

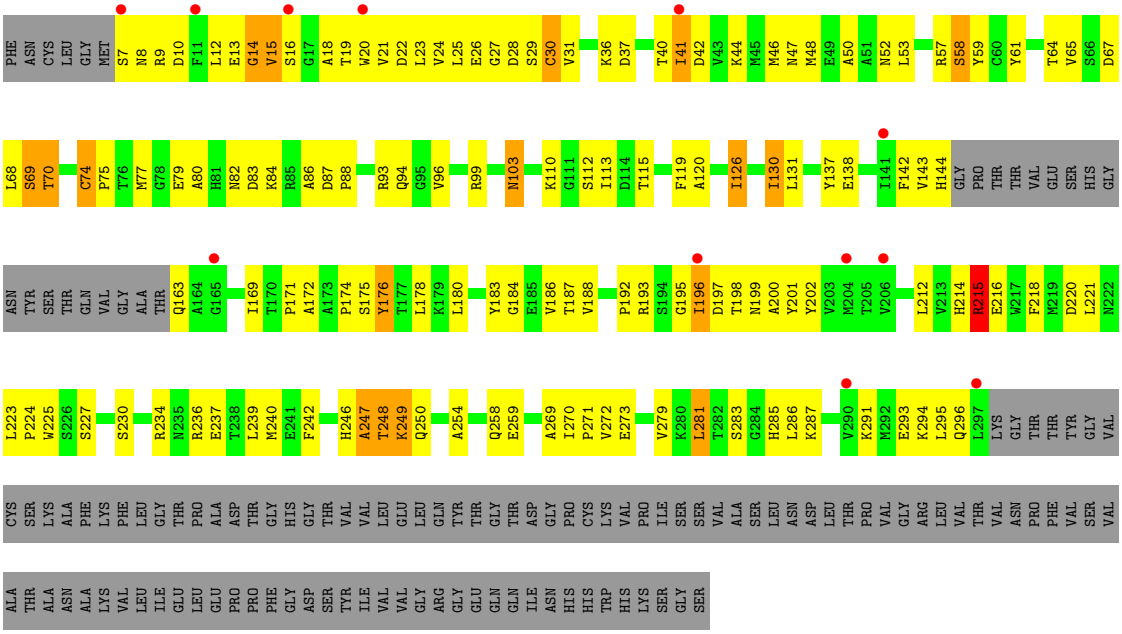
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Envelope glycoprotein

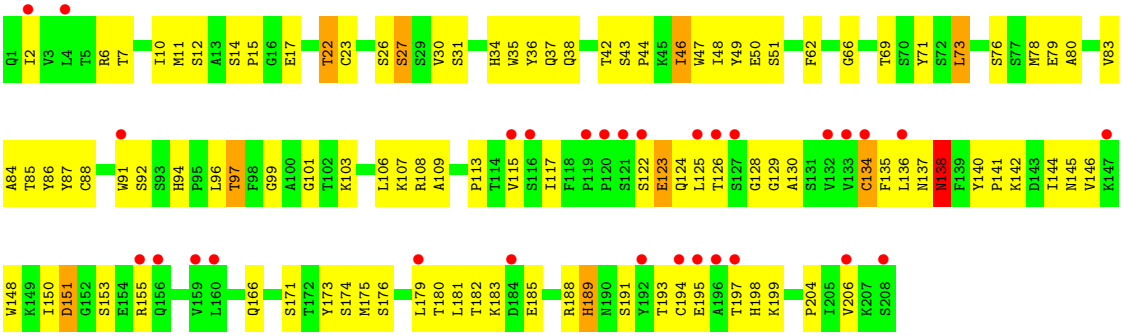
Chain E:





• Molecule 2: murine kappa light chain of E53 monoclonal antibody Fab

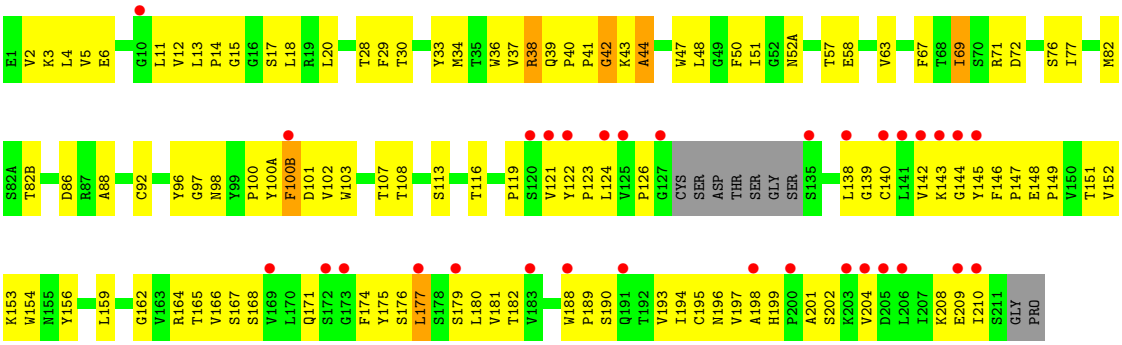
Chain L:



• Molecule 3: murine heavy chain (IgG3) of E53 monoclonal antibody Fab

Chain H:

14%
45%
48%


E1 V2 K3 L4 V5 E6 G10 L11 V12 L13 P14 G15 G16 S17 L18 R19 L20 T28 F29 T30 Y33 M34 T35 W36 V37 R38 Q39 P40 P41 G42 K43 A44 W47 L48 G49 F50 I51 G52 N52A T57 E58 V63 F67 T68 I69 S70 R71 D72 S76 I77 M82
S82A T82B D86 R87 A88 C92 Y96 G97 N98 Y99 P100 Y100A F100B D101 V102 W103 T107 T108 S113 T116 P119 S120 V121 Y122 P123 L124 V125 P126 G127 CYS SER ASP THR SER GLY SER S135 L138 G139 C140 L141 V142 K143 G144 Y145 F146 P147 E148 P149 V150 T151 V152
K153 W154 N155 Y156 L159 G162 V163 R164 T165 V166 S167 S168 V169 L170 Q171 S172 G173 F174 Y175 S176 L177 S178 S179 L180 V181 T182 V183 W188 P189 S190 Q191 T192 V193 I194 C195 N196 V197 A198 H199 P200 A201 S202 K203 V204 D205 L206 I207 K208 E209 I210 S211 GLY PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	146.41Å 160.14Å 43.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 50.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (20.00-3.00) 99.3 (50.15-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.01Å)	Xtriage
Refinement program	PHENIX ?	Depositor
R, R_{free}	0.247 , 0.344 0.261 , 0.346	Depositor DCC
R_{free} test set	1097 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	100.7	Xtriage
Anisotropy	0.893	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 106.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5283	wwPDB-VP
Average B, all atoms (Å^2)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	E	0.26	0/2128	0.48	0/2878
2	L	0.29	0/1620	0.49	0/2198
3	H	0.27	0/1654	0.50	0/2262
All	All	0.27	0/5402	0.49	0/7338

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2088	0	2057	121	0
2	L	1583	0	1522	104	0
3	H	1612	0	1584	109	0
All	All	5283	0	5163	322	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 31.

All (322) 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:E:79:GLU:HG2	1:E:94:GLN:HE22	1.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:168:SER:HB3	3:H:177:LEU:HB3	1.48	0.93
1:E:26:GLU:HG3	1:E:28:ASP:H	1.33	0.90
3:H:51:ILE:HD13	3:H:71:ARG:HG3	1.54	0.89
1:E:42:ASP:HB2	1:E:142:PHE:HB2	1.55	0.88
3:H:148:GLU:HG2	3:H:149:PRO:HA	1.57	0.86
1:E:215:ARG:HH11	1:E:215:ARG:CG	1.90	0.84
1:E:79:GLU:HG2	1:E:94:GLN:NE2	1.93	0.83
1:E:53:LEU:HD22	1:E:130:ILE:HG12	1.59	0.83
2:L:103:LYS:HE3	3:H:43:LYS:HD2	1.58	0.83
1:E:19:THR:HB	1:E:293:GLU:HB2	1.59	0.82
1:E:46:MET:HB2	1:E:138:GLU:HB3	1.63	0.80
1:E:25:LEU:O	1:E:285:HIS:HB2	1.81	0.80
3:H:37:VAL:HG22	3:H:47:TRP:HA	1.62	0.79
1:E:77:MET:HE2	3:H:98:ASN:H	1.48	0.78
1:E:224:PRO:HG2	1:E:239:LEU:HD12	1.65	0.78
2:L:155:ARG:HD3	2:L:179:LEU:HD21	1.65	0.78
1:E:59:TYR:CD2	1:E:225:TRP:HB3	2.18	0.78
3:H:199:HIS:NE2	3:H:201:ALA:HB3	1.99	0.77
1:E:23:LEU:HD11	1:E:31:VAL:HG21	1.66	0.77
3:H:143:LYS:HB3	3:H:143:LYS:HZ2	1.49	0.77
1:E:9:ARG:HG3	1:E:30:CYS:SG	2.24	0.77
1:E:77:MET:HE2	3:H:98:ASN:N	1.99	0.77
2:L:195:GLU:HA	2:L:206:VAL:HG22	1.65	0.77
1:E:15:VAL:HG12	1:E:18:ALA:HB3	1.68	0.75
1:E:248:THR:HG23	1:E:249:LYS:H	1.52	0.74
2:L:122:SER:HA	2:L:125:LEU:HD12	1.70	0.73
2:L:124:GLN:HG2	2:L:129:GLY:HA3	1.70	0.73
2:L:6:ARG:NH2	2:L:88:CYS:H	1.87	0.73
2:L:128:GLY:HA2	2:L:183:LYS:HD2	1.72	0.72
1:E:215:ARG:HH11	1:E:215:ARG:HG3	1.52	0.71
3:H:13:LEU:HD22	3:H:113:SER:HA	1.74	0.70
1:E:44:LYS:HD2	1:E:46:MET:SD	2.32	0.70
1:E:23:LEU:HD21	1:E:31:VAL:HB	1.74	0.69
1:E:65:VAL:HG23	1:E:254:ALA:HB2	1.74	0.69
3:H:208:LYS:HG2	3:H:209:GLU:H	1.57	0.69
1:E:61:TYR:HB2	1:E:258:GLN:HB2	1.74	0.69
2:L:46:ILE:HD13	2:L:47:TRP:N	2.08	0.69
2:L:155:ARG:HH22	2:L:181:LEU:CD1	2.05	0.69
2:L:37:GLN:HG3	2:L:86:TYR:CE1	2.28	0.68
1:E:26:GLU:CG	1:E:29:SER:H	2.06	0.68
2:L:181:LEU:HD23	2:L:182:THR:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:154:TRP:CZ3	3:H:195:CYS:HB3	2.29	0.68
1:E:26:GLU:HG2	1:E:29:SER:H	1.57	0.68
1:E:30:CYS:HB3	1:E:44:LYS:HG3	1.76	0.67
2:L:155:ARG:NH2	2:L:181:LEU:HB2	2.10	0.67
2:L:46:ILE:HD13	2:L:47:TRP:H	1.59	0.67
1:E:23:LEU:HD12	1:E:24:VAL:H	1.60	0.66
1:E:26:GLU:HG2	1:E:29:SER:HB3	1.77	0.66
1:E:14:GLY:O	1:E:21:VAL:HG22	1.95	0.66
3:H:29:PHE:CD2	3:H:76:SER:HA	2.31	0.66
2:L:6:ARG:NH1	2:L:86:TYR:O	2.28	0.66
2:L:7:THR:HB	2:L:22:THR:HB	1.78	0.66
2:L:125:LEU:HD23	2:L:130:ALA:HB2	1.77	0.65
3:H:3:LYS:HE2	3:H:5:VAL:HG12	1.79	0.65
2:L:78:MET:O	2:L:79:GLU:HG3	1.97	0.65
3:H:123:PRO:HA	3:H:210:ILE:HD12	1.78	0.65
2:L:47:TRP:HZ3	2:L:62:PHE:CE2	2.14	0.64
1:E:201:TYR:HB3	1:E:212:LEU:HD11	1.78	0.64
1:E:58:SER:HB3	1:E:126:ILE:HA	1.78	0.64
2:L:155:ARG:HH22	2:L:181:LEU:HD13	1.61	0.64
2:L:183:LYS:C	2:L:185:GLU:H	2.00	0.64
2:L:183:LYS:C	2:L:183:LYS:HD3	2.19	0.64
2:L:185:GLU:HG3	2:L:188:ARG:HB3	1.79	0.63
3:H:3:LYS:HE2	3:H:5:VAL:CG1	2.29	0.63
3:H:51:ILE:HG23	3:H:71:ARG:HD2	1.80	0.63
2:L:47:TRP:CZ3	2:L:62:PHE:CE2	2.86	0.62
3:H:143:LYS:HZ3	3:H:144:GLY:H	1.47	0.62
1:E:26:GLU:HG2	1:E:29:SER:CB	2.30	0.61
2:L:135:PHE:CE2	3:H:180:LEU:HD11	2.35	0.61
3:H:38:ARG:HG2	3:H:48:LEU:HD21	1.83	0.61
2:L:150:ILE:HB	2:L:153:SER:HB2	1.83	0.61
2:L:185:GLU:HA	2:L:188:ARG:HB3	1.81	0.61
1:E:13:GLU:O	1:E:14:GLY:C	2.39	0.61
3:H:121:VAL:HG22	3:H:142:VAL:HG22	1.83	0.60
2:L:6:ARG:HH21	2:L:99:GLY:HA3	1.67	0.60
1:E:59:TYR:CE2	1:E:225:TRP:HB3	2.36	0.60
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.36	0.60
3:H:67:PHE:CD1	3:H:82:MET:HA	2.36	0.60
2:L:103:LYS:CE	3:H:43:LYS:HD2	2.31	0.60
3:H:143:LYS:HG2	3:H:176:SER:OG	2.02	0.60
2:L:94:HIS:NE2	3:H:58:GLU:HG2	2.16	0.59
3:H:100(B):PHE:CD1	3:H:100(B):PHE:N	2.69	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:66:GLY:HA3	2:L:71:TYR:CD2	2.37	0.59
2:L:73:LEU:C	2:L:73:LEU:HD12	2.23	0.59
2:L:12:SER:HB3	2:L:107:LYS:HB2	1.85	0.59
1:E:12:LEU:HD13	1:E:31:VAL:HG11	1.85	0.58
2:L:155:ARG:HH21	2:L:181:LEU:HB2	1.68	0.58
2:L:108:ARG:HG3	2:L:109:ALA:O	2.03	0.58
2:L:142:LYS:HB2	2:L:173:TYR:CE2	2.39	0.58
3:H:188:TRP:CD1	3:H:193:VAL:HG21	2.39	0.58
1:E:70:THR:HB	1:E:115:THR:OG1	2.04	0.58
2:L:183:LYS:C	2:L:185:GLU:N	2.58	0.58
1:E:70:THR:HG21	1:E:250:GLN:H	1.69	0.57
1:E:169:ILE:HD12	1:E:174:PRO:O	2.04	0.57
2:L:36:TYR:CE1	2:L:46:ILE:HG12	2.39	0.57
3:H:100(A):TYR:HE1	3:H:101:ASP:HB3	1.69	0.57
3:H:72:ASP:HB3	3:H:77:ILE:HB	1.87	0.57
3:H:100(B):PHE:N	3:H:100(B):PHE:HD1	2.01	0.57
1:E:143:VAL:O	1:E:163:GLN:HG2	2.05	0.57
2:L:6:ARG:HH12	2:L:101:GLY:HA2	1.70	0.57
1:E:223:LEU:O	1:E:225:TRP:HD1	1.87	0.57
1:E:193:ARG:HD2	1:E:287:LYS:NZ	2.20	0.56
2:L:145:ASN:HB2	2:L:197:THR:HG23	1.87	0.56
1:E:14:GLY:O	1:E:15:VAL:HG23	2.05	0.56
3:H:148:GLU:HB2	3:H:175:TYR:CZ	2.40	0.56
2:L:37:GLN:HG3	2:L:86:TYR:CZ	2.41	0.56
2:L:91:TRP:CZ2	3:H:100:PRO:HG2	2.41	0.56
3:H:40:PRO:HD2	3:H:44:ALA:O	2.06	0.56
2:L:47:TRP:HZ3	2:L:62:PHE:CZ	2.22	0.56
1:E:53:LEU:HD11	1:E:279:VAL:HG21	1.88	0.56
1:E:272:VAL:HG12	1:E:273:GLU:N	2.20	0.56
2:L:47:TRP:CZ3	2:L:62:PHE:CZ	2.94	0.56
3:H:33:TYR:O	3:H:34:MET:HG2	2.06	0.56
3:H:179:SER:C	3:H:180:LEU:HD12	2.26	0.56
2:L:175:MET:HG2	2:L:176:SER:N	2.21	0.55
3:H:152:VAL:HA	3:H:196:ASN:O	2.06	0.55
3:H:199:HIS:CD2	3:H:202:SER:H	2.25	0.55
2:L:107:LYS:HA	2:L:140:TYR:OH	2.07	0.55
2:L:198:HIS:CG	2:L:199:LYS:H	2.25	0.55
1:E:96:VAL:HG13	1:E:110:LYS:HD2	1.88	0.54
2:L:150:ILE:HD11	2:L:155:ARG:HD2	1.88	0.54
3:H:152:VAL:HG22	3:H:197:VAL:HG13	1.88	0.54
1:E:215:ARG:HH11	1:E:215:ARG:HG2	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:ARG:HH22	2:L:87:TYR:HA	1.72	0.54
1:E:200:ALA:O	1:E:215:ARG:HB2	2.08	0.54
3:H:188:TRP:CD1	3:H:189:PRO:HA	2.42	0.54
2:L:179:LEU:HD12	2:L:180:THR:H	1.73	0.54
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.90	0.54
3:H:41:PRO:HD3	3:H:88:ALA:HA	1.89	0.54
1:E:15:VAL:CG1	1:E:18:ALA:HB3	2.37	0.53
3:H:63:VAL:HG12	3:H:63:VAL:O	2.06	0.53
1:E:64:THR:OG1	1:E:120:ALA:HB3	2.09	0.53
2:L:128:GLY:C	2:L:183:LYS:HB3	2.28	0.53
2:L:151:ASP:OD2	2:L:189:HIS:CD2	2.60	0.53
3:H:101:ASP:O	3:H:103:TRP:HD1	1.90	0.53
1:E:175:SER:O	1:E:176:TYR:HB2	2.08	0.53
1:E:19:THR:HB	1:E:293:GLU:CB	2.34	0.53
1:E:53:LEU:CD2	1:E:130:ILE:HG12	2.37	0.53
2:L:73:LEU:HD12	2:L:73:LEU:O	2.07	0.53
3:H:100(A):TYR:CE1	3:H:101:ASP:HB3	2.44	0.53
3:H:15:GLY:O	3:H:82(B):THR:HA	2.09	0.52
3:H:29:PHE:CG	3:H:76:SER:HA	2.45	0.52
3:H:156:TYR:H	3:H:196:ASN:HD21	1.57	0.52
1:E:7:SER:C	1:E:9:ARG:H	2.13	0.52
1:E:269:ALA:O	1:E:271:PRO:HD3	2.09	0.52
2:L:140:TYR:CG	2:L:141:PRO:HA	2.45	0.52
2:L:47:TRP:HZ3	2:L:62:PHE:CD2	2.28	0.52
3:H:177:LEU:O	3:H:177:LEU:HD12	2.09	0.52
1:E:187:THR:HB	1:E:291:LYS:HB2	1.90	0.52
1:E:172:ALA:O	1:E:174:PRO:HD3	2.10	0.51
1:E:291:LYS:HB3	1:E:294:LYS:HE2	1.92	0.51
2:L:91:TRP:CE2	3:H:100:PRO:HD2	2.45	0.51
3:H:36:TRP:CD1	3:H:69:ILE:HD12	2.46	0.51
2:L:123:GLU:HB3	3:H:122:TYR:CE1	2.45	0.51
1:E:93:ARG:HG3	1:E:242:PHE:CE1	2.46	0.51
1:E:270:ILE:O	1:E:272:VAL:HG23	2.11	0.51
3:H:36:TRP:HD1	3:H:69:ILE:HD12	1.76	0.51
3:H:116:THR:HG23	3:H:201:ALA:HB1	1.92	0.50
1:E:193:ARG:HD2	1:E:287:LYS:HZ3	1.75	0.50
2:L:117:ILE:HD12	2:L:194:CYS:SG	2.51	0.50
1:E:224:PRO:HA	1:E:234:ARG:O	2.11	0.50
2:L:150:ILE:CD1	2:L:155:ARG:HD2	2.40	0.50
3:H:124:LEU:HB2	3:H:139:GLY:O	2.11	0.50
1:E:131:LEU:HD21	1:E:199:ASN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:103:TRP:CD1	3:H:103:TRP:N	2.79	0.50
3:H:202:SER:O	3:H:204:VAL:HG13	2.12	0.50
1:E:65:VAL:HG22	1:E:240:MET:HE2	1.94	0.50
2:L:137:ASN:HD22	3:H:164:ARG:HG3	1.77	0.49
2:L:150:ILE:HG12	2:L:155:ARG:HD2	1.94	0.49
3:H:50:PHE:O	3:H:57:THR:HG23	2.12	0.49
3:H:153:LYS:HB2	3:H:196:ASN:HB2	1.94	0.49
3:H:143:LYS:NZ	3:H:144:GLY:H	2.10	0.49
3:H:188:TRP:HA	3:H:190:SER:H	1.77	0.49
1:E:96:VAL:CG1	1:E:110:LYS:HD2	2.42	0.49
3:H:28:THR:HG22	3:H:28:THR:O	2.11	0.49
1:E:200:ALA:O	1:E:201:TYR:HD1	1.95	0.49
1:E:24:VAL:O	1:E:25:LEU:HD23	2.12	0.49
2:L:155:ARG:NH2	2:L:181:LEU:CB	2.76	0.49
3:H:194:ILE:HG22	3:H:209:GLU:HB3	1.95	0.49
1:E:216:GLU:O	1:E:220:ASP:HB2	2.13	0.48
1:E:15:VAL:HB	1:E:20:TRP:O	2.13	0.48
1:E:180:LEU:HB2	1:E:184:GLY:O	2.13	0.48
1:E:202:TYR:O	1:E:212:LEU:HD12	2.13	0.48
1:E:246:HIS:O	1:E:247:ALA:C	2.52	0.48
1:E:26:GLU:HG3	1:E:27:GLY:N	2.29	0.48
3:H:147:PRO:HD2	3:H:201:ALA:HB1	1.96	0.47
1:E:196:ILE:HG12	1:E:197:ASP:N	2.29	0.47
2:L:2:ILE:O	2:L:97:THR:HG21	2.14	0.47
2:L:124:GLN:C	2:L:126:THR:H	2.16	0.47
1:E:23:LEU:HD21	1:E:31:VAL:CB	2.44	0.47
2:L:108:ARG:HG3	2:L:109:ALA:N	2.29	0.47
3:H:17:SER:HB2	3:H:82:MET:O	2.14	0.47
3:H:38:ARG:NH2	3:H:86:ASP:HA	2.30	0.47
1:E:40:THR:OG1	1:E:144:HIS:ND1	2.47	0.47
1:E:214:HIS:O	1:E:215:ARG:C	2.54	0.47
2:L:73:LEU:C	2:L:73:LEU:CD1	2.83	0.47
1:E:57:ARG:HD2	1:E:225:TRP:CE3	2.50	0.47
3:H:143:LYS:HB3	3:H:143:LYS:NZ	2.24	0.47
3:H:171:GLN:O	3:H:174:PHE:HB2	2.14	0.46
2:L:14:SER:O	2:L:17:GLU:HB3	2.15	0.46
2:L:15:PRO:HG3	2:L:106:LEU:HD11	1.97	0.46
3:H:96:TYR:O	3:H:100:PRO:HA	2.16	0.46
3:H:139:GLY:HA3	3:H:179:SER:O	2.15	0.46
1:E:24:VAL:HA	1:E:286:LEU:O	2.15	0.46
1:E:84:LYS:HD3	1:E:84:LYS:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:2:VAL:CG1	3:H:102:VAL:HG11	2.46	0.46
3:H:148:GLU:CG	3:H:149:PRO:HA	2.36	0.46
3:H:101:ASP:O	3:H:103:TRP:CD1	2.68	0.46
1:E:215:ARG:CG	1:E:215:ARG:NH1	2.61	0.46
1:E:258:GLN:O	1:E:259:GLU:C	2.53	0.46
3:H:67:PHE:HD1	3:H:82:MET:HA	1.78	0.46
1:E:10:ASP:HB2	1:E:31:VAL:HG22	1.96	0.46
1:E:57:ARG:O	1:E:218:PHE:HZ	1.99	0.46
2:L:150:ILE:CG1	2:L:155:ARG:HD2	2.46	0.46
2:L:7:THR:HB	2:L:22:THR:CB	2.44	0.46
2:L:26:SER:O	2:L:27:SER:HB2	2.16	0.46
3:H:12:VAL:HG21	3:H:18:LEU:HD22	1.98	0.45
3:H:199:HIS:CE1	3:H:201:ALA:HB3	2.49	0.45
1:E:119:PHE:CG	1:E:236:ARG:HD2	2.50	0.45
3:H:51:ILE:HG23	3:H:51:ILE:O	2.15	0.45
1:E:183:TYR:O	1:E:296:GLN:HB3	2.16	0.45
2:L:130:ALA:N	2:L:183:LYS:HB2	2.31	0.45
3:H:38:ARG:HH21	3:H:86:ASP:HA	1.81	0.45
1:E:50:ALA:HB1	1:E:53:LEU:HD21	1.99	0.45
1:E:84:LYS:C	1:E:86:ALA:H	2.20	0.45
1:E:80:ALA:H	1:E:112:SER:CB	2.30	0.45
3:H:166:VAL:HG23	3:H:167:SER:O	2.15	0.45
2:L:36:TYR:CD1	2:L:46:ILE:HA	2.51	0.45
1:E:53:LEU:HD11	1:E:279:VAL:CG2	2.46	0.45
1:E:193:ARG:NH1	1:E:287:LYS:HE2	2.32	0.45
1:E:295:LEU:HD12	1:E:296:GLN:H	1.82	0.45
3:H:6:GLU:HB3	3:H:107:THR:HB	1.99	0.45
1:E:41:ILE:HG22	1:E:143:VAL:HG22	1.99	0.44
1:E:285:HIS:NE2	1:E:287:LYS:HD2	2.33	0.44
2:L:166:GLN:HG3	2:L:171:SER:O	2.17	0.44
3:H:154:TRP:CH2	3:H:195:CYS:HB3	2.52	0.44
1:E:48:MET:HE2	1:E:281:LEU:HB2	2.00	0.44
1:E:183:TYR:O	1:E:295:LEU:HD12	2.17	0.44
3:H:199:HIS:HD2	3:H:202:SER:OG	2.01	0.44
3:H:63:VAL:HG13	3:H:67:PHE:CD2	2.53	0.44
2:L:38:GLN:O	2:L:84:ALA:HB1	2.18	0.44
3:H:181:VAL:HG22	3:H:182:THR:N	2.33	0.44
1:E:137:TYR:CE2	1:E:192:PRO:HB3	2.52	0.44
2:L:194:CYS:O	2:L:206:VAL:HA	2.18	0.44
1:E:202:TYR:HE1	1:E:215:ARG:HD2	1.83	0.43
2:L:14:SER:O	2:L:17:GLU:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:121:VAL:HG12	3:H:208:LYS:HD2	1.99	0.43
1:E:50:ALA:HB1	1:E:130:ILE:HG21	2.00	0.43
1:E:50:ALA:CB	1:E:130:ILE:HD13	2.47	0.43
1:E:215:ARG:HG3	1:E:215:ARG:NH1	2.26	0.43
1:E:74:CYS:HB3	1:E:75:PRO:HD2	2.00	0.43
2:L:42:THR:HG22	2:L:43:SER:O	2.18	0.43
3:H:30:THR:O	3:H:52(A):ASN:HB2	2.18	0.43
3:H:165:THR:HA	3:H:179:SER:HA	2.00	0.43
1:E:200:ALA:C	1:E:201:TYR:HD1	2.21	0.43
2:L:137:ASN:O	2:L:138:ASN:C	2.56	0.43
1:E:12:LEU:HD13	1:E:31:VAL:CG1	2.48	0.43
1:E:93:ARG:HG3	1:E:242:PHE:CZ	2.54	0.43
2:L:10:ILE:HG12	2:L:11:MET:N	2.34	0.43
3:H:140:CYS:SG	3:H:210:ILE:HD11	2.59	0.43
1:E:227:SER:H	1:E:230:SER:HB3	1.82	0.43
2:L:85:THR:HG23	2:L:103:LYS:HD3	2.00	0.42
2:L:151:ASP:N	2:L:151:ASP:OD1	2.52	0.42
3:H:63:VAL:O	3:H:63:VAL:CG1	2.67	0.42
3:H:71:ARG:HE	3:H:71:ARG:HB3	1.68	0.42
1:E:47:ASN:O	1:E:138:GLU:N	2.51	0.42
1:E:195:GLY:HA3	1:E:283:SER:HB2	2.00	0.42
3:H:96:TYR:CD2	3:H:97:GLY:N	2.87	0.42
3:H:119:PRO:HG3	3:H:145:TYR:CB	2.49	0.42
1:E:246:HIS:O	1:E:248:THR:N	2.53	0.42
2:L:6:ARG:NH2	2:L:87:TYR:HA	2.33	0.42
3:H:2:VAL:HG11	3:H:102:VAL:HG11	2.01	0.42
2:L:197:THR:HB	2:L:204:PRO:HB3	2.00	0.42
1:E:13:GLU:O	1:E:13:GLU:HG3	2.19	0.42
3:H:168:SER:HA	3:H:176:SER:O	2.19	0.42
1:E:175:SER:HA	1:E:188:VAL:O	2.19	0.42
2:L:129:GLY:C	2:L:183:LYS:HG3	2.40	0.42
2:L:138:ASN:HD21	3:H:164:ARG:HH11	1.68	0.42
3:H:188:TRP:CA	3:H:190:SER:H	2.32	0.42
1:E:197:ASP:O	1:E:200:ALA:HB3	2.18	0.42
2:L:80:ALA:O	2:L:83:VAL:HG23	2.19	0.42
1:E:193:ARG:HH11	1:E:287:LYS:HE2	1.85	0.41
2:L:135:PHE:CD2	3:H:180:LEU:HD11	2.54	0.41
2:L:135:PHE:C	2:L:136:LEU:HD12	2.41	0.41
1:E:68:LEU:HD12	1:E:68:LEU:HA	1.83	0.41
1:E:70:THR:HG21	1:E:250:GLN:N	2.33	0.41
1:E:99:ARG:NH1	1:E:103:ASN:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:47:TRP:CZ3	2:L:62:PHE:CD2	3.08	0.41
2:L:96:LEU:N	2:L:96:LEU:HD23	2.34	0.41
2:L:30:VAL:CG1	2:L:31:SER:N	2.84	0.41
2:L:134:CYS:HB2	2:L:148:TRP:CH2	2.55	0.41
2:L:115:VAL:HA	2:L:135:PHE:O	2.20	0.41
1:E:83:ASP:OD1	1:E:83:ASP:N	2.54	0.41
1:E:171:PRO:HA	1:E:192:PRO:HG2	2.02	0.41
2:L:142:LYS:O	2:L:144:ILE:HG22	2.21	0.41
2:L:151:ASP:CG	2:L:191:SER:HB2	2.40	0.41
3:H:116:THR:HA	3:H:146:PHE:O	2.21	0.41
1:E:169:ILE:HG23	1:E:174:PRO:HA	2.02	0.41
2:L:146:VAL:HG21	2:L:175:MET:SD	2.61	0.41
1:E:87:ASP:HA	1:E:88:PRO:HD3	1.94	0.41
2:L:6:ARG:NH1	2:L:101:GLY:HA2	2.35	0.41
2:L:50:GLU:O	2:L:51:SER:HB2	2.21	0.41
3:H:3:LYS:HE2	3:H:5:VAL:HG11	2.03	0.41
3:H:11:LEU:HB2	3:H:147:PRO:HG3	2.03	0.41
3:H:42:GLY:O	3:H:43:LYS:HB2	2.21	0.41
3:H:142:VAL:HB	3:H:177:LEU:HD12	2.03	0.41
3:H:145:TYR:CZ	3:H:175:TYR:HB2	2.56	0.41
2:L:34:HIS:HD2	2:L:49:TYR:HA	1.86	0.41
3:H:126:PRO:HD3	3:H:138:LEU:HG	2.03	0.41
2:L:34:HIS:CD2	2:L:49:TYR:HA	2.56	0.40
3:H:138:LEU:HB3	3:H:139:GLY:H	1.72	0.40
3:H:151:THR:OG1	3:H:198:ALA:HB3	2.21	0.40
3:H:164:ARG:N	3:H:180:LEU:O	2.42	0.40
2:L:6:ARG:NE	2:L:88:CYS:SG	2.95	0.40
3:H:162:GLY:O	3:H:181:VAL:HA	2.21	0.40
1:E:69:SER:O	1:E:82:ASN:ND2	2.54	0.40
3:H:39:GLN:O	3:H:88:ALA:HB1	2.21	0.40
3:H:188:TRP:HA	3:H:190:SER:N	2.36	0.40
1:E:236:ARG:O	1:E:237:GLU:C	2.59	0.40
1:E:221:LEU:HD23	1:E:221:LEU:HA	1.97	0.40
2:L:6:ARG:NH2	2:L:99:GLY:HA3	2.34	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	E	269/402 (67%)	207 (77%)	51 (19%)	11 (4%)	3 16
2	L	205/207 (99%)	164 (80%)	36 (18%)	5 (2%)	6 29
3	H	208/221 (94%)	174 (84%)	31 (15%)	3 (1%)	11 43
All	All	682/830 (82%)	545 (80%)	118 (17%)	19 (3%)	5 25

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	16	SER
1	E	215	ARG
1	E	14	GLY
1	E	36	LYS
1	E	52	ASN
1	E	69	SER
1	E	247	ALA
2	L	27	SER
2	L	44	PRO
2	L	138	ASN
1	E	176	TYR
1	E	248	THR
2	L	174	SER
3	H	42	GLY
3	H	44	ALA
1	E	8	ASN
3	H	14	PRO
2	L	113	PRO
1	E	74	CYS

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	E	226/332 (68%)	207 (92%)	19 (8%)	11	38
2	L	182/182 (100%)	169 (93%)	13 (7%)	14	46
3	H	180/187 (96%)	171 (95%)	9 (5%)	24	60
All	All	588/701 (84%)	547 (93%)	41 (7%)	15	47

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	15	VAL
1	E	22	ASP
1	E	30	CYS
1	E	37	ASP
1	E	41	ILE
1	E	58	SER
1	E	67	ASP
1	E	70	THR
1	E	103	ASN
1	E	113	ILE
1	E	126	ILE
1	E	130	ILE
1	E	178	LEU
1	E	186	VAL
1	E	196	ILE
1	E	198	THR
1	E	215	ARG
1	E	249	LYS
1	E	281	LEU
2	L	22	THR
2	L	46	ILE
2	L	69	THR
2	L	73	LEU
2	L	76	SER
2	L	92	SER
2	L	97	THR

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Mol	Chain	Res	Type
2	L	123	GLU
2	L	134	CYS
2	L	138	ASN
2	L	151	ASP
2	L	189	HIS
2	L	193	THR
3	H	4	LEU
3	H	20	LEU
3	H	38	ARG
3	H	69	ILE
3	H	92	CYS
3	H	100(B)	PHE
3	H	108	THR
3	H	159	LEU
3	H	177	LEU

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

Mol	Chain	Res	Type
1	E	94	GLN
2	L	1	GLN
2	L	34	HIS
2	L	137	ASN
3	H	196	ASN
3	H	199	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	E	273/402 (67%)	0.38	12 (4%)	34	13	70, 130, 191, 236	0
2	L	207/207 (100%)	0.88	30 (14%)	2	1	66, 134, 229, 275	0
3	H	212/221 (95%)	0.88	32 (15%)	2	1	67, 148, 276, 316	0
All	All	692/830 (83%)	0.68	74 (10%)	6	2	66, 135, 244, 316	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	120	PRO	12.4
2	L	155	ARG	10.3
3	H	127	GLY	9.8
3	H	138	LEU	7.7
3	H	198	ALA	6.9
3	H	205	ASP	6.2
2	L	194	CYS	5.6
3	H	121	VAL	5.0
1	E	11	PHE	5.0
2	L	121	SER	5.0
3	H	142	VAL	4.9
3	H	183	VAL	4.9
2	L	208	SER	4.5
2	L	192	TYR	4.1
1	E	297	LEU	3.9
2	L	127	SER	3.9
2	L	195	GLU	3.9
1	E	165	GLY	3.8
2	L	132	VAL	3.8
2	L	156	GLN	3.8
3	H	120	SER	3.7
3	H	145	TYR	3.7
3	H	177	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	L	115	VAL	3.6
2	L	126	THR	3.6
3	H	200	PRO	3.6
1	E	20	TRP	3.4
3	H	143	LYS	3.3
2	L	125	LEU	3.2
3	H	122	TYR	3.2
3	H	172	SER	3.2
2	L	159	VAL	3.2
2	L	122	SER	3.1
3	H	135	SER	3.1
3	H	125	VAL	3.1
3	H	206	LEU	3.0
2	L	196	ALA	3.0
2	L	197	THR	2.9
2	L	133	VAL	2.8
3	H	144	GLY	2.8
2	L	147	LYS	2.7
3	H	10	GLY	2.7
3	H	173	GLY	2.7
1	E	290	VAL	2.6
3	H	141	LEU	2.6
2	L	136	LEU	2.6
3	H	204	VAL	2.6
2	L	91	TRP	2.5
1	E	16	SER	2.5
3	H	169	VAL	2.5
2	L	179	LEU	2.4
3	H	209	GLU	2.3
3	H	210	ILE	2.3
3	H	124	LEU	2.3
1	E	206	VAL	2.3
3	H	188	TRP	2.3
1	E	204	MET	2.3
1	E	196	ILE	2.3
3	H	179	SER	2.3
2	L	4	LEU	2.2
3	H	203	LYS	2.2
3	H	140	CYS	2.2
1	E	7	SER	2.2
2	L	206	VAL	2.2
3	H	100(B)	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	2	ILE	2.2
2	L	184	ASP	2.1
2	L	119	PRO	2.1
1	E	41	ILE	2.1
2	L	116	SER	2.1
1	E	141	ILE	2.0
3	H	191	GLN	2.0
2	L	134	CYS	2.0
2	L	160	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.