



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:46 AM GMT

PDB ID : 3FZU
Title : IgG1 Fab characterized by H/D exchange
Authors : Arndt, J.; Houde, D.; Domeier, W.; Berkowitz, S.; Engen, J.R.
Deposited on : 2009-01-26
Resolution : 2.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

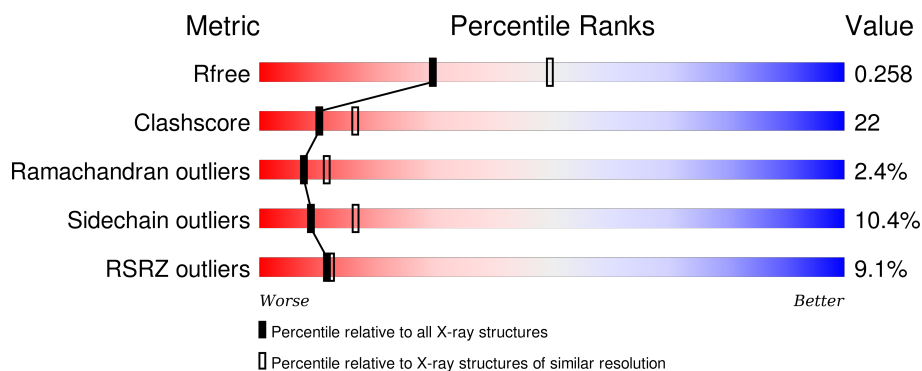
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	D	214	<div> <div>10%</div> <div> <div></div> <div>56%</div> <div>34%</div> <div>8%</div> <div>.</div> </div> </div>
1	L	214	<div> <div>6%</div> <div> <div></div> <div>54%</div> <div>41%</div> <div>.</div> <div>.</div> </div> </div>
2	C	223	<div> <div>12%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>5%</div> <div>.</div> </div> </div>
2	H	223	<div> <div>8%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>5%</div> <div>.</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6540 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 immunoglobulin IgG1 Fab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1648	1033	277	333	5			
1	D	213	Total	C	N	O	S	0	0	0
			1630	1023	275	327	5			

- Molecule 2 is a protein called immunoglobulin IgG1 Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1611	1015	273	317	6			
2	C	214	Total	C	N	O	S	0	0	0
			1596	1007	270	313	6			

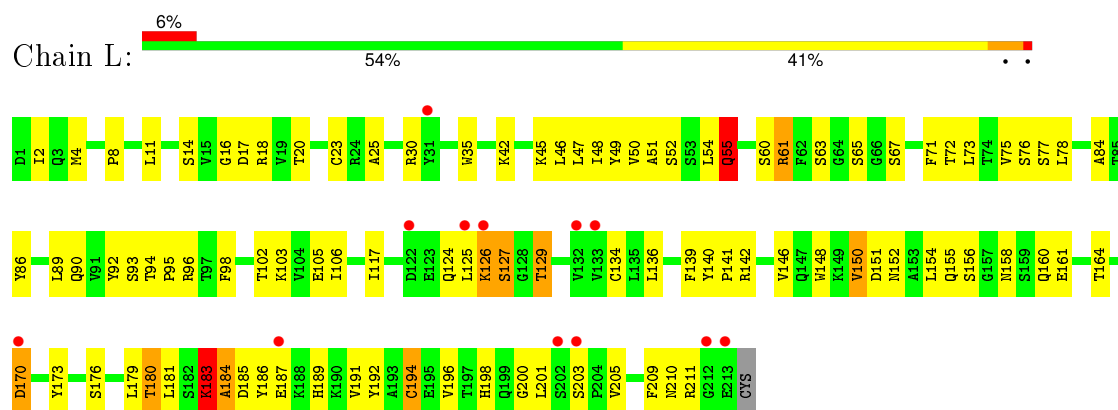
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	7	Total	O	0	0
			7	7		
3	D	15	Total	O	0	0
			15	15		
3	H	12	Total	O	0	0
			12	12		
3	L	21	Total	O	0	0
			21	21		

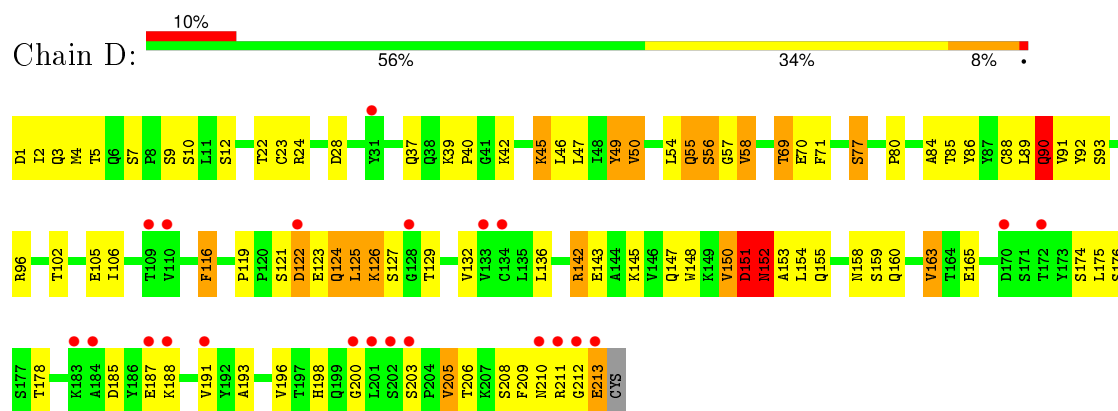
3 Residue-property plots

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.

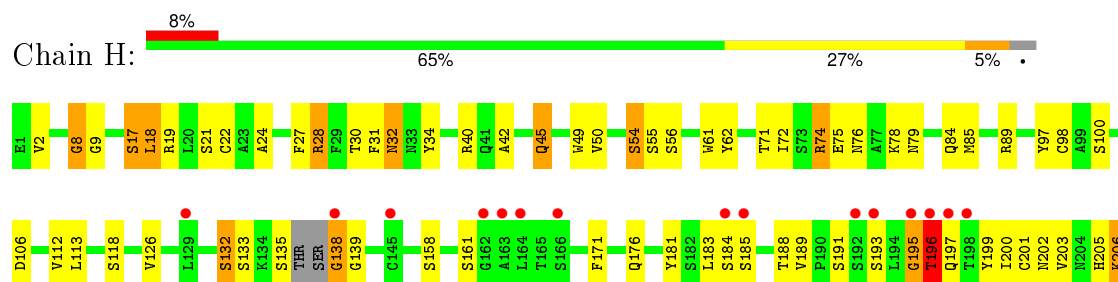
- Molecule 1: immunoglobulin IgG1 Fab, light chain

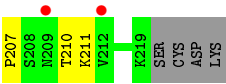


- Molecule 1: immunoglobulin IgG1 Fab, light chain

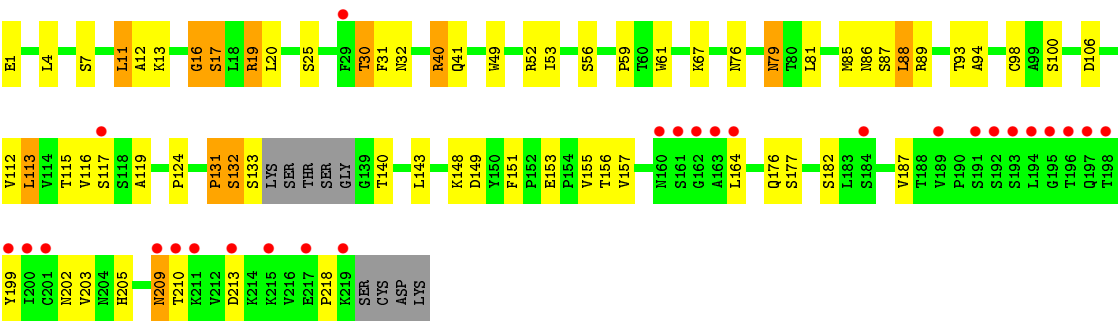


- Molecule 2: immunoglobulin IgG1 Fab, heavy chain





● Molecule 2: immunoglobulin IgG1 Fab, heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	243.05Å 61.94Å 100.85Å 90.00° 113.94° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 33.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-2.50) 93.9 (33.28-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.261 0.220 , 0.258	Depositor DCC
R_{free} test set	2293 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 70.0	EDS
Estimated twinning fraction	0.048 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 45004 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6540	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	D	1.45	9/1665 (0.5%)	1.03	1/2264 (0.0%)
1	L	1.54	6/1683 (0.4%)	1.10	3/2285 (0.1%)
2	C	1.39	0/1634	0.97	2/2226 (0.1%)
2	H	1.34	4/1649 (0.2%)	1.00	3/2246 (0.1%)
All	All	1.43	19/6631 (0.3%)	1.03	9/9021 (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	D	0	1
2	H	0	2
All	All	0	3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	62	TYR	CD2-CE2	-5.99	1.30	1.39
1	L	16	GLY	C-O	-5.86	1.14	1.23
1	D	143	GLU	CG-CD	5.53	1.60	1.51
1	D	91	VAL	CB-CG2	5.51	1.64	1.52
1	L	76	SER	CB-OG	-5.50	1.35	1.42
1	D	49	TYR	CD2-CE2	-5.42	1.31	1.39
2	H	61	TRP	CG-CD1	-5.36	1.29	1.36
1	L	194	CYS	CB-SG	-5.33	1.73	1.81
1	D	71	PHE	CD1-CE1	-5.32	1.28	1.39
1	D	88	CYS	CB-SG	-5.32	1.73	1.81
1	L	103	LYS	CE-NZ	5.29	1.62	1.49
1	L	49	TYR	CD2-CE2	-5.16	1.31	1.39
1	D	92	TYR	CD1-CE1	5.15	1.47	1.39
1	L	42	LYS	CE-NZ	5.14	1.61	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	58	VAL	CB-CG2	-5.13	1.42	1.52
2	H	62	TYR	CD1-CE1	-5.12	1.31	1.39
1	D	142	ARG	CB-CG	-5.11	1.38	1.52
1	D	213	GLU	CB-CG	5.10	1.61	1.52
2	H	181	TYR	CD2-CE2	-5.00	1.31	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	61	ARG	N-CA-CB	-5.86	100.04	110.60
1	L	170	ASP	CB-CG-OD1	-5.83	113.06	118.30
2	H	8	GLY	N-CA-C	-5.76	98.71	113.10
2	C	1	GLU	N-CA-C	-5.61	95.86	111.00
2	C	81	LEU	CB-CG-CD1	-5.28	102.02	111.00
1	D	90	GLN	N-CA-CB	-5.26	101.13	110.60
1	L	55	GLN	CA-CB-CG	-5.14	102.10	113.40
2	H	89	ARG	CB-CA-C	5.08	120.57	110.40
2	H	196	THR	N-CA-CB	5.03	119.86	110.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	151	ASP	Peptide
2	H	138	GLY	Peptide
2	H	97	TYR	Peptide

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	D	1630	0	1581	87	0
1	L	1648	0	1613	87	0
2	C	1596	0	1558	58	0
2	H	1611	0	1570	57	0
3	C	7	0	0	1	0
3	D	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	12	0	0	1	0
3	L	21	0	0	0	0
All	All	6540	0	6322	275	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 22.

All (275) 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:C:11:LEU:HD12	2:C:12:ALA:N	1.34	1.37
1:D:150:VAL:HG23	1:D:155:GLN:NE2	1.35	1.35
1:D:121:SER:HB2	1:D:122:ASP:CB	1.67	1.22
1:D:122:ASP:CB	1:D:123:GLU:CB	2.30	1.09
1:L:124:GLN:HE21	1:L:129:THR:HG22	1.10	1.06
1:L:124:GLN:NE2	1:L:129:THR:HG22	1.75	1.01
1:L:150:VAL:HG13	1:L:192:TYR:CD1	1.97	0.98
2:H:30:THR:HG23	2:H:32:ASN:HD21	1.32	0.94
1:D:150:VAL:CG2	1:D:155:GLN:NE2	2.30	0.94
2:C:11:LEU:CD1	2:C:12:ALA:N	2.30	0.93
1:D:50:VAL:HG23	1:D:50:VAL:O	1.70	0.92
2:H:30:THR:HG23	2:H:32:ASN:ND2	1.84	0.92
1:L:134:CYS:SG	1:L:194:CYS:CB	2.59	0.90
1:L:150:VAL:CG1	1:L:192:TYR:CE1	2.55	0.88
2:C:79:ASN:HD22	2:C:79:ASN:N	1.71	0.88
1:D:2:ILE:HG22	1:D:4:MET:HE2	1.56	0.88
2:C:11:LEU:HD12	2:C:12:ALA:H	1.06	0.88
2:C:131:PRO:O	2:C:132:SER:HB2	1.74	0.86
1:D:150:VAL:HG23	1:D:155:GLN:HE21	1.34	0.86
1:L:124:GLN:HE21	1:L:129:THR:CG2	1.89	0.85
2:C:11:LEU:CD1	2:C:12:ALA:H	1.89	0.84
1:D:121:SER:CB	1:D:122:ASP:CB	2.53	0.84
1:D:191:VAL:HG22	1:D:210:ASN:OD1	1.81	0.80
1:D:55:GLN:HE21	1:D:55:GLN:HA	1.45	0.80
1:L:136:LEU:N	1:L:136:LEU:HD12	1.96	0.79
2:C:157:VAL:HG22	2:C:203:VAL:HG22	1.66	0.78
2:C:131:PRO:O	2:C:132:SER:CB	2.30	0.78
2:H:32:ASN:H	2:H:32:ASN:HD22	1.31	0.77
2:H:195:GLY:CA	2:H:196:THR:HG22	2.14	0.77
2:C:11:LEU:HD12	2:C:11:LEU:C	2.04	0.77
2:C:30:THR:CG2	2:C:32:ASN:HB2	2.14	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:THR:HG22	2:C:32:ASN:HB2	1.67	0.76
2:H:195:GLY:N	2:H:196:THR:HG22	2.01	0.75
1:L:2:ILE:HG22	1:L:4:MET:CE	2.17	0.74
1:D:2:ILE:HG22	1:D:4:MET:CE	2.18	0.73
1:L:150:VAL:HG13	1:L:192:TYR:CE1	2.23	0.72
2:H:42:ALA:HB3	2:H:45:GLN:HG3	1.71	0.72
2:C:19:ARG:HG2	2:C:19:ARG:HH11	1.54	0.72
2:C:19:ARG:HG2	2:C:19:ARG:NH1	2.04	0.71
1:L:65:SER:HB3	1:L:72:THR:HG23	1.72	0.71
2:C:79:ASN:HD22	2:C:79:ASN:H	1.37	0.71
2:H:195:GLY:HA3	2:H:196:THR:HG22	1.72	0.71
2:C:30:THR:HG23	2:C:32:ASN:ND2	2.05	0.71
1:D:150:VAL:HG23	1:D:155:GLN:CD	2.10	0.71
1:L:150:VAL:CG1	1:L:192:TYR:CD1	2.74	0.70
1:L:2:ILE:HG22	1:L:4:MET:HE3	1.71	0.70
1:D:142:ARG:HH21	1:D:163:VAL:HG11	1.57	0.69
1:D:24:ARG:NE	1:D:70:GLU:OE2	2.23	0.69
1:L:124:GLN:NE2	1:L:129:THR:CG2	2.53	0.67
1:L:4:MET:HE2	1:L:25:ALA:HA	1.75	0.67
1:L:150:VAL:HG11	1:L:192:TYR:CE1	2.30	0.67
2:C:131:PRO:HG3	2:C:143:LEU:HB3	1.76	0.67
1:L:180:THR:O	1:L:180:THR:HG22	1.94	0.67
1:L:96:ARG:HG3	2:H:49:TRP:CD1	2.29	0.67
1:L:198:HIS:CD2	1:L:200:GLY:H	2.13	0.67
1:D:175:LEU:C	1:D:175:LEU:HD23	2.14	0.67
2:H:195:GLY:HA3	2:H:196:THR:CB	2.24	0.66
1:D:2:ILE:HD12	1:D:93:SER:HB3	1.78	0.66
2:H:195:GLY:HA3	2:H:196:THR:CG2	2.25	0.66
2:C:119:ALA:HB3	2:C:151:PHE:CE1	2.29	0.66
1:D:50:VAL:CG2	1:D:50:VAL:O	2.41	0.66
1:D:123:GLU:O	1:D:125:LEU:N	2.29	0.65
1:D:125:LEU:C	1:D:127:SER:H	1.99	0.65
2:H:193:SER:O	2:H:196:THR:CG2	2.45	0.65
2:C:93:THR:HG23	2:C:115:THR:HA	1.77	0.65
1:L:125:LEU:C	1:L:127:SER:H	1.99	0.65
2:H:32:ASN:N	2:H:32:ASN:HD22	1.94	0.65
2:C:19:ARG:HG3	2:C:20:LEU:N	2.12	0.65
1:D:28:ASP:C	1:D:28:ASP:OD1	2.35	0.65
2:H:30:THR:CG2	2:H:32:ASN:HD21	2.08	0.65
1:D:150:VAL:H	1:D:155:GLN:HE21	1.45	0.65
1:D:123:GLU:O	1:D:126:LYS:N	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:GLY:HA3	2:H:196:THR:HB	1.79	0.64
1:L:125:LEU:O	1:L:127:SER:N	2.30	0.64
2:H:31:PHE:CD2	2:H:79:ASN:HA	2.33	0.64
1:D:153:ALA:O	1:D:155:GLN:NE2	2.30	0.64
1:D:151:ASP:O	1:D:153:ALA:N	2.30	0.63
1:L:136:LEU:CD1	1:L:136:LEU:N	2.61	0.63
2:C:30:THR:HG23	2:C:32:ASN:HD22	1.63	0.63
1:D:125:LEU:O	1:D:127:SER:N	2.30	0.62
1:D:123:GLU:O	1:D:124:GLN:C	2.37	0.62
1:L:125:LEU:C	1:L:127:SER:N	2.51	0.62
2:H:18:LEU:HB2	2:H:85:MET:HE3	1.80	0.62
1:L:50:VAL:O	1:L:51:ALA:HB3	1.99	0.62
1:L:90:GLN:HE21	1:L:92:TYR:H	1.46	0.62
1:L:198:HIS:HD2	1:L:200:GLY:H	1.46	0.62
2:H:19:ARG:HG3	2:H:84:GLN:NE2	2.15	0.61
1:D:2:ILE:CD1	1:D:93:SER:HB3	2.30	0.61
1:D:80:PRO:HA	1:D:106:ILE:HD13	1.83	0.61
1:L:61:ARG:HG2	1:L:75:VAL:HG13	1.83	0.60
2:C:13:LYS:O	2:C:16:GLY:N	2.30	0.59
2:H:22:CYS:SG	2:H:98:CYS:CB	2.92	0.57
2:H:161:SER:H	2:H:202:ASN:HD21	1.52	0.57
2:H:100:SER:O	2:H:106:ASP:HA	2.05	0.56
2:H:189:VAL:HG11	2:H:199:TYR:CE2	2.39	0.56
1:D:212:GLY:O	1:D:213:GLU:HG3	2.05	0.56
1:D:4:MET:HE3	1:D:90:GLN:HG3	1.88	0.56
2:C:132:SER:OG	2:C:133:SER:N	2.29	0.56
2:H:139:GLY:C	2:H:191:SER:HG	2.09	0.56
2:C:148:LYS:O	2:C:149:ASP:HB2	2.04	0.55
2:C:19:ARG:HH11	2:C:19:ARG:CG	2.20	0.55
2:H:135:SER:O	2:H:138:GLY:N	2.39	0.55
2:C:30:THR:C	2:C:32:ASN:H	2.10	0.55
2:C:4:LEU:HD13	2:C:98:CYS:SG	2.46	0.55
1:D:55:GLN:HE21	1:D:55:GLN:CA	2.18	0.55
1:D:187:GLU:HA	1:D:211:ARG:CZ	2.36	0.55
2:C:49:TRP:CD1	1:D:96:ARG:CG	2.90	0.55
2:C:30:THR:O	2:C:32:ASN:N	2.39	0.54
1:D:119:PRO:HB3	1:D:209:PHE:CZ	2.42	0.54
2:H:210:THR:HG22	2:H:211:LYS:N	2.21	0.54
2:C:79:ASN:ND2	2:C:79:ASN:N	2.45	0.54
2:H:158:SER:OG	2:H:202:ASN:ND2	2.35	0.54
2:H:183:LEU:HD12	2:H:183:LEU:C	2.27	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:PRO:O	1:L:102:THR:HG23	2.06	0.54
1:D:4:MET:CE	1:D:90:GLN:HG3	2.38	0.54
1:D:158:ASN:OD1	1:D:158:ASN:N	2.39	0.54
1:L:146:VAL:HG22	1:L:196:VAL:HG22	1.89	0.54
1:L:2:ILE:CG2	1:L:4:MET:HE1	2.38	0.54
1:D:77:SER:OG	1:D:77:SER:O	2.26	0.54
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.44	0.53
1:D:124:GLN:O	1:D:127:SER:N	2.41	0.53
2:C:17:SER:OG	2:C:86:ASN:OD1	2.27	0.53
1:L:46:LEU:HD23	1:L:55:GLN:HG3	1.90	0.53
2:H:193:SER:O	2:H:196:THR:HG22	2.08	0.53
2:H:132:SER:OG	2:H:133:SER:N	2.40	0.53
1:D:125:LEU:C	1:D:127:SER:N	2.61	0.53
1:D:198:HIS:CD2	1:D:200:GLY:H	2.26	0.53
2:C:30:THR:C	2:C:32:ASN:N	2.62	0.53
1:D:55:GLN:NE2	1:D:55:GLN:HA	2.20	0.52
1:L:2:ILE:HG22	1:L:4:MET:HE1	1.88	0.52
1:D:145:LYS:HE3	1:D:147:GLN:NE2	2.25	0.52
1:D:136:LEU:HD11	1:D:196:VAL:HG21	1.91	0.52
1:D:210:ASN:HB2	1:D:213:GLU:OE1	2.09	0.52
1:D:116:PHE:N	1:D:116:PHE:CD1	2.77	0.52
1:D:193:ALA:HB2	1:D:208:SER:HB3	1.92	0.52
2:C:124:PRO:HD2	2:C:210:THR:HG21	1.92	0.52
2:C:32:ASN:HA	2:C:76:ASN:ND2	2.23	0.52
2:C:49:TRP:CD1	1:D:96:ARG:HG2	2.44	0.51
1:L:61:ARG:HD2	1:L:77:SER:O	2.10	0.51
1:D:2:ILE:CG2	1:D:4:MET:CE	2.87	0.51
1:D:145:LYS:O	1:D:196:VAL:HA	2.11	0.51
2:C:88:LEU:HB3	2:C:116:VAL:HG21	1.91	0.51
1:L:180:THR:O	1:L:180:THR:CG2	2.55	0.50
1:L:90:GLN:NE2	1:L:93:SER:H	2.09	0.50
2:C:209:ASN:C	2:C:209:ASN:HD22	2.13	0.50
2:C:40:ARG:HG2	2:C:41:GLN:N	2.26	0.50
2:H:210:THR:CG2	2:H:211:LYS:N	2.75	0.50
1:D:205:VAL:HG13	1:D:206:THR:N	2.26	0.50
2:H:32:ASN:CB	2:H:76:ASN:ND2	2.75	0.50
1:D:193:ALA:HB1	1:D:206:THR:HG23	1.93	0.50
2:C:87:SER:O	2:C:88:LEU:O	2.30	0.50
2:H:126:VAL:CG2	2:H:203:VAL:HG21	2.42	0.50
2:C:93:THR:O	2:C:94:ALA:HB2	2.12	0.49
2:C:89:ARG:O	2:C:116:VAL:HG11	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:ARG:HG2	1:L:75:VAL:CG1	2.42	0.49
1:D:150:VAL:O	1:D:151:ASP:O	2.30	0.49
1:L:89:LEU:HD13	1:L:98:PHE:CE2	2.48	0.49
1:L:65:SER:HB3	1:L:72:THR:CG2	2.41	0.49
1:L:150:VAL:HG11	1:L:192:TYR:HE1	1.78	0.49
1:L:183:LYS:O	1:L:184:ALA:C	2.48	0.49
1:D:187:GLU:O	1:D:211:ARG:NH2	2.46	0.49
1:D:175:LEU:HD23	1:D:176:SER:N	2.27	0.48
1:L:160:GLN:HE22	2:H:176:GLN:HG2	1.77	0.48
2:H:193:SER:O	2:H:196:THR:HG23	2.13	0.48
2:C:87:SER:O	2:C:88:LEU:C	2.52	0.48
1:D:89:LEU:HD11	1:D:96:ARG:HB3	1.95	0.48
1:D:150:VAL:O	1:D:151:ASP:C	2.52	0.48
1:L:150:VAL:HG23	1:L:155:GLN:NE2	2.29	0.48
1:L:48:ILE:CD1	1:L:54:LEU:HD12	2.44	0.48
2:H:161:SER:N	2:H:202:ASN:HD21	2.11	0.48
1:D:124:GLN:O	1:D:125:LEU:C	2.51	0.48
2:H:17:SER:HA	2:H:85:MET:O	2.13	0.48
1:L:50:VAL:O	1:L:51:ALA:CB	2.61	0.48
1:L:96:ARG:HG3	2:H:49:TRP:CG	2.49	0.47
1:L:18:ARG:NH2	1:D:70:GLU:OE1	2.46	0.47
2:H:28:ARG:HB2	2:H:28:ARG:HE	1.40	0.47
2:H:2:VAL:HG21	2:H:27:PHE:CE2	2.50	0.47
1:D:145:LYS:HE3	1:D:147:GLN:HE22	1.79	0.47
2:C:113:LEU:HD13	3:C:248:HOH:O	2.15	0.47
1:L:141:PRO:O	1:L:198:HIS:HE1	1.96	0.47
1:L:117:ILE:HD13	1:L:209:PHE:HD1	1.80	0.47
2:C:20:LEU:HD11	2:C:85:MET:HE1	1.95	0.47
1:L:187:GLU:O	1:L:211:ARG:NH2	2.48	0.47
2:H:32:ASN:ND2	2:H:32:ASN:H	2.07	0.47
1:L:201:LEU:HD13	1:L:205:VAL:HG23	1.97	0.47
2:C:143:LEU:HD21	2:C:199:TYR:CD1	2.50	0.46
2:H:196:THR:HG23	2:H:197:GLN:N	2.29	0.46
1:L:90:GLN:NE2	1:L:92:TYR:H	2.13	0.46
1:L:186:TYR:CE1	1:L:192:TYR:CE2	3.02	0.46
1:L:160:GLN:NE2	2:H:176:GLN:HG2	2.31	0.46
1:L:94:THR:HA	1:L:95:PRO:C	2.36	0.46
2:H:139:GLY:C	2:H:191:SER:OG	2.54	0.46
1:L:63:SER:O	1:L:73:LEU:HD12	2.16	0.46
2:H:75:GLU:OE2	2:H:78:LYS:HD2	2.16	0.46
1:D:185:ASP:OD1	1:D:188:LYS:NZ	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:PRO:CB	1:D:165:GLU:HG2	2.46	0.46
1:L:185:ASP:N	1:L:185:ASP:OD1	2.43	0.46
1:L:11:LEU:HD12	1:L:11:LEU:C	2.37	0.46
1:L:170:ASP:OD1	1:L:170:ASP:C	2.54	0.46
1:D:5:THR:O	1:D:5:THR:HG22	2.15	0.46
1:D:54:LEU:HD11	1:D:58:VAL:HG12	1.97	0.46
2:H:34:TYR:O	2:H:74:ARG:NH2	2.40	0.45
1:D:159:SER:HA	1:D:178:THR:O	2.17	0.45
1:D:148:TRP:O	1:D:155:GLN:HG2	2.17	0.45
2:H:24:ALA:HB1	2:H:27:PHE:HE1	1.81	0.45
1:L:67:SER:HA	1:L:71:PHE:CE2	2.52	0.45
1:D:119:PRO:HB3	1:D:209:PHE:CE2	2.52	0.45
1:D:152:ASN:N	1:D:152:ASN:OD1	2.47	0.45
1:D:37:GLN:OE1	1:D:39:LYS:HE3	2.17	0.44
1:L:158:ASN:O	1:L:179:LEU:HD12	2.17	0.44
2:C:155:VAL:HG12	2:C:205:HIS:CD2	2.53	0.44
2:C:59:PRO:HG2	2:C:61:TRP:CH2	2.52	0.44
2:C:30:THR:CG2	2:C:32:ASN:CB	2.91	0.44
1:L:84:ALA:HB3	1:L:86:TYR:CE1	2.52	0.44
2:C:164:LEU:CD2	2:C:187:VAL:HG21	2.47	0.44
2:C:88:LEU:HB3	2:C:116:VAL:CG2	2.47	0.44
1:L:14:SER:O	1:L:17:ASP:HB2	2.18	0.44
1:L:106:ILE:N	1:L:106:ILE:HD13	2.32	0.44
1:L:90:GLN:HE22	1:L:93:SER:H	1.65	0.43
2:H:72:ILE:O	3:H:226:HOH:O	2.21	0.43
1:L:89:LEU:HD13	1:L:98:PHE:CD2	2.54	0.43
1:D:37:GLN:HB2	1:D:47:LEU:HD11	2.00	0.43
2:C:100:SER:O	2:C:106:ASP:HA	2.18	0.43
1:D:46:LEU:HD21	1:D:49:TYR:HB3	2.00	0.43
1:D:175:LEU:CD2	1:D:175:LEU:C	2.84	0.43
1:L:142:ARG:HB2	1:L:173:TYR:CE2	2.53	0.43
1:D:85:THR:HA	1:D:102:THR:O	2.18	0.43
2:H:40:ARG:HD3	2:H:50:VAL:CG2	2.49	0.43
2:C:88:LEU:HA	2:C:88:LEU:HD23	1.63	0.43
2:H:22:CYS:HG	2:H:98:CYS:HG	0.45	0.43
2:C:53:ILE:HG23	2:C:53:ILE:O	2.19	0.43
2:H:206:LYS:N	2:H:207:PRO:CD	2.81	0.43
1:D:150:VAL:O	1:D:153:ALA:HB3	2.19	0.43
1:L:18:ARG:HD3	1:D:22:THR:HG21	2.00	0.43
1:D:84:ALA:HB3	1:D:86:TYR:CE1	2.54	0.42
1:L:4:MET:HE2	1:L:25:ALA:CA	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:164:THR:HG23	2:H:171:PHE:CE2	2.55	0.42
1:L:154:LEU:O	1:D:154:LEU:HD23	2.18	0.42
2:H:18:LEU:HB2	2:H:85:MET:CE	2.47	0.42
1:L:78:LEU:HD21	1:L:106:ILE:HD12	2.02	0.42
1:L:154:LEU:HD23	1:D:154:LEU:HD21	2.01	0.42
1:L:17:ASP:HB3	1:D:7:SER:OG	2.20	0.42
1:L:105:GLU:HG2	1:L:106:ILE:N	2.34	0.42
1:L:186:TYR:HE1	1:L:192:TYR:CE2	2.38	0.42
1:D:56:SER:HA	1:D:57:GLY:HA2	1.82	0.42
1:D:22:THR:CG2	1:D:23:CYS:N	2.82	0.42
2:H:8:GLY:O	2:H:112:VAL:HG21	2.18	0.42
2:H:40:ARG:HD3	2:H:50:VAL:HG22	2.02	0.42
1:L:151:ASP:OD2	1:L:189:HIS:ND1	2.48	0.42
1:D:210:ASN:CB	1:D:213:GLU:OE1	2.68	0.42
1:D:119:PRO:HA	1:D:132:VAL:HG13	2.01	0.42
2:C:176:GLN:HA	1:D:160:GLN:NE2	2.35	0.42
1:D:69:THR:HG22	1:D:70:GLU:HG2	2.01	0.41
2:C:30:THR:HG23	2:C:32:ASN:H	1.85	0.41
2:C:17:SER:HA	2:C:85:MET:O	2.19	0.41
1:L:125:LEU:O	1:L:126:LYS:C	2.58	0.41
1:L:78:LEU:CD2	1:L:106:ILE:HD12	2.50	0.41
1:D:45:LYS:HD2	1:D:45:LYS:HA	1.81	0.41
1:L:71:PHE:N	1:L:71:PHE:CD1	2.89	0.41
1:L:136:LEU:CD1	1:L:136:LEU:H	2.30	0.41
2:C:205:HIS:HB3	2:C:210:THR:HB	2.01	0.41
2:H:78:LYS:O	2:H:79:ASN:C	2.58	0.41
1:L:140:TYR:CD1	1:L:141:PRO:HA	2.56	0.41
2:H:158:SER:OG	2:H:202:ASN:HB2	2.20	0.41
2:C:49:TRP:CD1	1:D:96:ARG:HG3	2.55	0.41
2:C:87:SER:C	2:C:88:LEU:O	2.57	0.41
1:L:139:PHE:CD1	1:L:139:PHE:N	2.89	0.41
1:L:136:LEU:HD21	1:L:146:VAL:CG2	2.51	0.40
2:H:54:SER:OG	2:H:55:SER:N	2.54	0.40
2:H:205:HIS:CD2	2:H:207:PRO:HD2	2.56	0.40
1:L:191:VAL:HG22	1:L:210:ASN:OD1	2.21	0.40
1:D:124:GLN:HG2	1:D:129:THR:O	2.22	0.40
1:L:201:LEU:HD23	1:L:201:LEU:HA	1.89	0.40
1:L:161:GLU:HA	1:L:176:SER:O	2.20	0.40
1:L:23:CYS:HB2	1:L:35:TRP:CH2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	D	211/214 (99%)	185 (88%)	20 (10%)	6 (3%)	6	9
1	L	211/214 (99%)	196 (93%)	11 (5%)	4 (2%)	10	16
2	C	210/223 (94%)	195 (93%)	9 (4%)	6 (3%)	6	8
2	H	213/223 (96%)	196 (92%)	13 (6%)	4 (2%)	10	16
All	All	845/874 (97%)	772 (91%)	53 (6%)	20 (2%)	7	11

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	132	SER
2	H	196	THR
2	C	132	SER
1	D	124	GLN
1	D	152	ASN
1	L	52	SER
2	H	195	GLY
1	D	122	ASP
1	D	126	LYS
1	L	126	LYS
2	C	31	PHE
1	D	125	LEU
1	D	151	ASP
1	L	183	LYS
1	L	184	ALA
2	C	16	GLY
2	C	218	PRO
2	C	88	LEU
2	C	131	PRO
2	H	9	GLY

5.3.2 Protein sidechains ⓘ

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	D	184/190 (97%)	163 (89%)	21 (11%)	7	13
1	L	189/190 (100%)	174 (92%)	15 (8%)	15	28
2	C	178/187 (95%)	156 (88%)	22 (12%)	6	11
2	H	179/187 (96%)	161 (90%)	18 (10%)	9	17
All	All	730/754 (97%)	654 (90%)	76 (10%)	9	16

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	THR
1	L	30	ARG
1	L	45	LYS
1	L	47	LEU
1	L	55	GLN
1	L	60	SER
1	L	127	SER
1	L	129	THR
1	L	150	VAL
1	L	152	ASN
1	L	156	SER
1	L	180	THR
1	L	181	LEU
1	L	183	LYS
1	L	203	SER
2	H	17	SER
2	H	18	LEU
2	H	21	SER
2	H	28	ARG
2	H	32	ASN
2	H	45	GLN
2	H	54	SER
2	H	56	SER
2	H	71	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	74	ARG
2	H	113	LEU
2	H	118	SER
2	H	184	SER
2	H	185	SER
2	H	188	THR
2	H	200	ILE
2	H	201	CYS
2	H	206	LYS
2	C	7	SER
2	C	11	LEU
2	C	17	SER
2	C	19	ARG
2	C	25	SER
2	C	30	THR
2	C	40	ARG
2	C	52	ARG
2	C	56	SER
2	C	67	LYS
2	C	79	ASN
2	C	112	VAL
2	C	113	LEU
2	C	117	SER
2	C	140	THR
2	C	153	GLU
2	C	156	THR
2	C	177	SER
2	C	182	SER
2	C	202	ASN
2	C	209	ASN
2	C	213	ASP
1	D	1	ASP
1	D	3	GLN
1	D	9	SER
1	D	10	SER
1	D	12	SER
1	D	42	LYS
1	D	45	LYS
1	D	50	VAL
1	D	55	GLN
1	D	56	SER
1	D	69	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	77	SER
1	D	90	GLN
1	D	105	GLU
1	D	116	PHE
1	D	150	VAL
1	D	152	ASN
1	D	163	VAL
1	D	174	SER
1	D	203	SER
1	D	205	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	90	GLN
1	L	124	GLN
1	L	152	ASN
1	L	198	HIS
2	H	32	ASN
2	H	84	GLN
2	H	202	ASN
2	C	32	ASN
2	C	79	ASN
2	C	209	ASN
1	D	55	GLN
1	D	124	GLN
1	D	147	GLN
1	D	155	GLN
1	D	160	GLN
1	D	198	HIS

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 [i](#)

There are no carbohydrates 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 ⓘ

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, 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	D	213/214 (99%)	0.68	22 (10%) 9 9	27, 39, 49, 54	0
1	L	213/214 (99%)	0.39	12 (5%) 28 31	24, 37, 48, 52	0
2	C	214/223 (95%)	0.70	27 (12%) 5 5	6, 24, 47, 52	0
2	H	217/223 (97%)	0.49	17 (7%) 16 17	18, 34, 45, 54	0
All	All	857/874 (98%)	0.57	78 (9%) 11 12	6, 36, 48, 54	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	210	ASN	8.1
2	C	163	ALA	8.1
2	C	198	THR	6.7
1	D	212	GLY	6.0
2	C	161	SER	6.0
2	C	162	GLY	5.6
2	C	197	GLN	5.5
1	D	191	VAL	5.4
1	D	213	GLU	5.1
2	C	193	SER	4.6
2	H	193	SER	4.4
2	C	192	SER	4.3
2	C	160	ASN	4.2
1	L	202	SER	4.1
2	C	211	LYS	4.0
2	C	196	THR	3.9
1	D	203	SER	3.7
1	D	184	ALA	3.7
2	C	195	GLY	3.6
2	C	164	LEU	3.6
2	H	184	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	192	SER	3.6
1	D	202	SER	3.6
2	H	163	ALA	3.5
2	H	196	THR	3.5
2	H	195	GLY	3.4
2	C	209	ASN	3.4
1	D	109	THR	3.2
1	D	187	GLU	3.1
2	H	197	GLN	3.1
1	L	203	SER	3.0
1	L	212	GLY	3.0
1	D	170	ASP	2.9
1	D	31	TYR	2.9
2	C	199	TYR	2.9
2	H	129	LEU	2.9
1	D	122	ASP	2.9
1	D	201	LEU	2.9
1	L	213	GLU	2.9
2	H	162	GLY	2.9
1	L	126	LYS	2.8
2	C	213	ASP	2.8
1	D	133	VAL	2.7
2	C	184	SER	2.7
2	C	194	LEU	2.6
2	H	164	LEU	2.6
1	D	128	GLY	2.6
1	L	187	GLU	2.6
2	C	189	VAL	2.5
1	D	134	CYS	2.5
1	L	170	ASP	2.5
2	C	217	GLU	2.5
2	H	166	SER	2.5
2	C	215	LYS	2.5
1	D	211	ARG	2.5
1	D	183	LYS	2.4
2	C	219	LYS	2.4
1	L	125	LEU	2.4
2	C	200	ILE	2.4
2	H	138	GLY	2.3
1	D	110	VAL	2.3
2	H	209	ASN	2.3
2	H	185	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	132	VAL	2.3
1	L	133	VAL	2.3
1	L	31	TYR	2.2
2	C	29	PHE	2.2
2	H	198	THR	2.2
2	H	212	VAL	2.2
2	C	201	CYS	2.2
2	C	117	SER	2.2
1	L	122	ASP	2.2
2	H	145	CYS	2.1
2	C	191	SER	2.1
1	D	200	GLY	2.0
1	D	172	THR	2.0
1	D	188	LYS	2.0
2	C	210	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.