Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:18 PM GMT

PDB ID	:	1A4J
Title	:	DIELS ALDER CATALYTIC ANTIBODY GERMLINE PRECURSOR
Authors	:	Spiller, B.W.; Romesburg, F.E.; Schultz, P.G.; Stevens, R.C.
Deposited on	:	1998-01-30
Resolution	:	2.10 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:

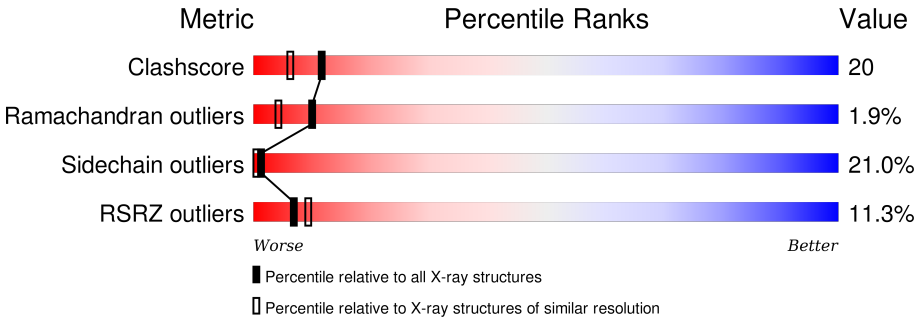
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	217	12% 54% 37% 8%
1	L	217	9% 53% 39% 7%
2	B	219	11% 56% 36% 5%
2	H	219	14% 57% 34% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6890 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, DIELS ALDER CATALYTIC ANTIBODY (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	0	0
			1668	1046	284	333	5			
1	A	217	Total	C	N	O	S	0	0	0
			1668	1046	284	333	5			

- Molecule 2 is a protein called IMMUNOGLOBULIN, DIELS ALDER CATALYTIC ANTIBODY (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1645	1046	271	322	6			
2	B	217	Total	C	N	O	S	0	0	0
			1645	1046	271	322	6			

- Molecule 3 is water.

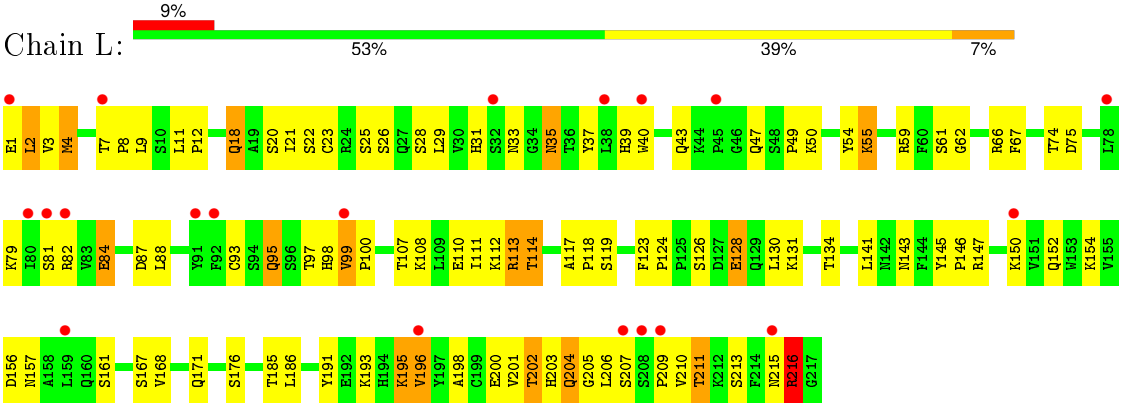
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	75	Total	O	0	0
			75	75		
3	H	86	Total	O	0	0
			86	86		
3	L	49	Total	O	0	0
			49	49		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

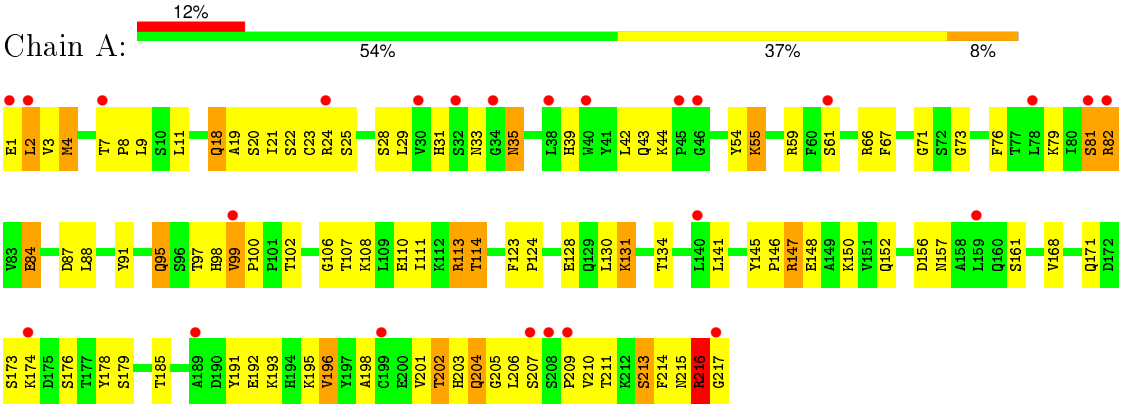
• Molecule 1: IMMUNOGLOBULIN, DIELS ALDER CATALYTIC ANTIBODY (LIGHT CHAIN)

Chain L:



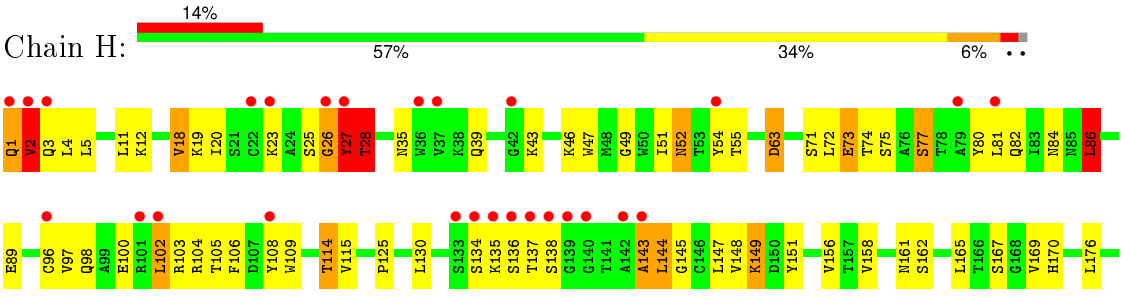
• Molecule 1: IMMUNOGLOBULIN, DIELS ALDER CATALYTIC ANTIBODY (LIGHT CHAIN)

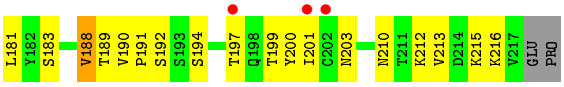
Chain A:



• Molecule 2: IMMUNOGLOBULIN, DIELS ALDER CATALYTIC ANTIBODY (HEAVY CHAIN)

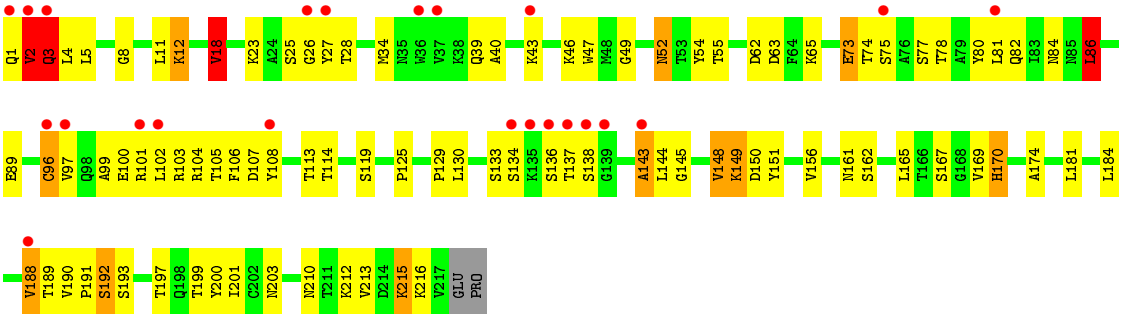
Chain H:





• Molecule 2: IMMUNOGLOBULIN, DIELS ALDER CATALYTIC ANTIBODY (HEAVY CHAIN)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.90Å 49.33Å 145.00Å 90.00° 108.74° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.10) 98.7 (19.89-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.09Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.229 , 0.292 0.243 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Outliers	2 of 61908 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6890	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.78 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.4445e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	A	0.39	0/1705	0.65	0/2312
1	L	0.39	0/1705	0.66	0/2312
2	B	0.47	0/1687	0.70	2/2298 (0.1%)
2	H	0.50	0/1687	0.72	1/2298 (0.0%)
All	All	0.44	0/6784	0.68	3/9220 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	18	VAL	CB-CA-C	-5.82	100.34	111.40
2	B	86	LEU	CA-CB-CG	5.23	127.34	115.30
2	H	86	LEU	CA-CB-CG	5.08	126.97	115.30

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	A	1668	0	1636	80	0
1	L	1668	0	1636	78	0
2	B	1645	0	1615	57	1
2	H	1645	0	1615	73	1
3	A	54	0	0	3	0
3	B	75	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	86	0	0	8	0
3	L	49	0	0	5	0
All	All	6890	0	6502	266	2

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 20.

All (266) 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:L:99:VAL:HB	1:L:100:PRO:HD3	1.21	1.11
1:A:99:VAL:HB	1:A:100:PRO:HD3	1.27	1.09
2:H:18:VAL:HG22	2:H:86:LEU:HD21	1.28	1.07
2:B:18:VAL:HG22	2:B:86:LEU:HD21	1.44	0.99
2:H:108:TYR:HB2	3:H:295:HOH:O	1.65	0.96
2:B:162:SER:H	2:B:203:ASN:HD21	1.16	0.89
1:L:99:VAL:HB	1:L:100:PRO:CD	2.05	0.87
2:B:12:LYS:HD2	2:B:18:VAL:HG13	1.58	0.86
1:L:21:ILE:HG12	1:L:107:THR:HG21	1.60	0.82
1:A:99:VAL:HB	1:A:100:PRO:CD	2.10	0.81
2:H:2:VAL:HG11	3:H:295:HOH:O	1.79	0.81
1:L:8:PRO:O	1:L:107:THR:HG23	1.82	0.80
2:H:162:SER:H	2:H:203:ASN:HD21	1.28	0.79
2:H:77:SER:HB2	3:H:291:HOH:O	1.84	0.77
1:A:21:ILE:HG12	1:A:107:THR:HG21	1.65	0.77
2:B:97:VAL:HG11	2:B:106:PHE:HB3	1.67	0.77
1:A:7:THR:HB	1:A:8:PRO:HD3	1.67	0.77
1:A:203:HIS:CD2	1:A:205:GLY:H	2.02	0.77
1:L:111:ILE:H	1:L:171:GLN:HE22	1.34	0.75
1:A:66:ARG:NH1	1:A:84:GLU:HG3	2.01	0.75
1:L:154:LYS:HE3	3:L:261:HOH:O	1.87	0.74
1:A:43:GLN:HE22	2:B:39:GLN:HE22	1.36	0.74
1:L:216:ARG:HH22	2:H:135:LYS:NZ	1.86	0.73
1:L:7:THR:HB	1:L:8:PRO:HD3	1.71	0.73
1:L:99:VAL:CB	1:L:100:PRO:HD3	2.12	0.72
2:H:52:ASN:HD22	2:H:54:TYR:H	1.37	0.72
1:L:39:HIS:CD2	2:H:105:THR:HG22	2.24	0.72
2:B:143:ALA:O	2:B:188:VAL:O	2.09	0.71
1:L:203:HIS:CD2	1:L:205:GLY:H	2.08	0.70
1:A:123:PHE:CZ	2:B:143:ALA:HB1	2.25	0.70
1:L:216:ARG:HH22	2:H:135:LYS:HZ1	1.36	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:ASP:HB2	3:H:296:HOH:O	1.92	0.70
2:B:52:ASN:HD22	2:B:54:TYR:H	1.40	0.69
1:L:123:PHE:CZ	2:H:143:ALA:HB1	2.26	0.69
2:H:52:ASN:ND2	2:H:54:TYR:H	1.89	0.68
2:B:129:PRO:HD3	2:B:215:LYS:HE2	1.75	0.67
2:H:12:LYS:HD2	2:H:18:VAL:HG13	1.78	0.66
2:H:52:ASN:HD21	2:H:54:TYR:HB3	1.59	0.66
2:H:143:ALA:O	2:H:188:VAL:O	2.14	0.66
1:A:31:HIS:HD2	1:A:33:ASN:H	1.43	0.65
2:B:52:ASN:ND2	2:B:54:TYR:H	1.94	0.65
1:A:146:PRO:HD2	1:A:204:GLN:HG2	1.79	0.65
1:A:113:ARG:HD3	1:A:114:THR:O	1.98	0.64
1:L:4:MET:HE2	1:L:23:CYS:SG	2.38	0.64
2:H:137:THR:O	2:H:192:SER:HB3	1.98	0.64
1:L:2:LEU:HG	1:L:26:SER:OG	1.98	0.63
1:L:143:ASN:HD21	2:H:170:HIS:CE1	2.15	0.63
1:A:2:LEU:HD21	1:A:29:LEU:HD21	1.81	0.62
1:L:146:PRO:HD2	1:L:204:GLN:HG2	1.80	0.62
2:B:129:PRO:HD3	2:B:215:LYS:CE	2.29	0.62
1:L:12:PRO:HA	1:L:110:GLU:HG3	1.81	0.62
2:B:169:VAL:HG22	2:B:188:VAL:HG13	1.82	0.62
1:L:198:ALA:HB2	1:L:213:SER:HB3	1.81	0.62
1:A:156:ASP:HA	1:A:196:VAL:HG23	1.82	0.62
2:H:149:LYS:HB2	2:H:183:SER:OG	2.00	0.62
1:A:215:ASN:O	1:A:217:GLY:N	2.34	0.61
2:H:191:PRO:HG2	2:H:194:SER:HB3	1.82	0.61
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.82	0.61
2:B:162:SER:N	2:B:203:ASN:HD21	1.93	0.61
1:L:100:PRO:HD2	3:L:252:HOH:O	1.99	0.61
1:A:99:VAL:CB	1:A:100:PRO:HD3	2.18	0.61
1:A:8:PRO:O	1:A:107:THR:HG23	2.00	0.61
1:A:179:SER:CB	2:B:170:HIS:HD2	2.14	0.61
2:H:2:VAL:HG12	2:H:98:GLN:OE1	2.02	0.60
2:B:162:SER:H	2:B:203:ASN:ND2	1.96	0.60
2:B:73:GLU:HB2	2:B:80:TYR:HE1	1.67	0.60
2:H:27:TYR:O	2:H:28:THR:HB	2.00	0.59
2:H:1:GLN:HB2	2:H:3:GLN:HG3	1.85	0.59
1:L:25:SER:CB	1:L:29:LEU:HD21	2.32	0.59
1:A:88:LEU:HD11	1:A:111:ILE:HG12	1.84	0.59
2:H:19:LYS:HD2	2:H:82:GLN:HE21	1.68	0.58
2:H:103:ARG:HH11	2:H:103:ARG:HG3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:LEU:HD13	1:L:210:VAL:HG23	1.85	0.58
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.39	0.58
1:L:31:HIS:HD2	1:L:33:ASN:H	1.49	0.58
2:B:100:GLU:HB2	2:B:107:ASP:OD2	2.04	0.58
1:A:4:MET:HE2	1:A:23:CYS:SG	2.43	0.58
1:A:18:GLN:HE22	1:A:79:LYS:HB3	1.69	0.58
1:A:111:ILE:H	1:A:171:GLN:HE22	1.51	0.57
2:B:137:THR:O	2:B:192:SER:HB3	2.04	0.57
2:B:52:ASN:ND2	2:B:55:THR:H	2.02	0.57
1:L:2:LEU:HD21	1:L:25:SER:HB2	1.87	0.57
1:L:156:ASP:HA	1:L:196:VAL:HG23	1.87	0.57
2:H:130:LEU:HD11	2:H:147:LEU:HB2	1.87	0.56
1:A:2:LEU:HD22	1:A:95:GLN:HG3	1.86	0.56
2:H:97:VAL:HG11	2:H:106:PHE:HB3	1.87	0.56
1:L:54:TYR:HD1	1:L:55:LYS:HG3	1.69	0.56
1:A:39:HIS:CD2	2:B:105:THR:HG22	2.40	0.56
1:L:25:SER:HB2	1:L:29:LEU:HD21	1.87	0.56
1:L:18:GLN:HE22	1:L:79:LYS:HB3	1.70	0.56
2:H:162:SER:N	2:H:203:ASN:HD21	2.00	0.56
2:B:4:LEU:HD12	2:B:108:TYR:HD1	1.70	0.56
2:H:18:VAL:HG22	2:H:86:LEU:CD2	2.19	0.55
2:B:52:ASN:HD21	2:B:54:TYR:HB3	1.70	0.55
1:A:123:PHE:HZ	2:B:143:ALA:HB1	1.68	0.55
2:B:99:ALA:HA	2:B:105:THR:O	2.06	0.55
2:H:51:ILE:HD13	2:H:72:LEU:HG	1.89	0.55
2:H:52:ASN:HD22	2:H:55:THR:H	1.54	0.55
1:A:2:LEU:HD13	1:A:98:HIS:CD2	2.42	0.55
2:B:134:SER:C	2:B:136:SER:H	2.10	0.55
2:B:34:MET:SD	2:B:96:CYS:SG	3.05	0.55
2:B:26:GLY:O	2:B:28:THR:N	2.35	0.55
1:A:206:LEU:HD13	1:A:210:VAL:HG23	1.88	0.54
2:H:73:GLU:HB2	2:H:80:TYR:HE1	1.72	0.54
1:L:88:LEU:HD11	1:L:111:ILE:HG12	1.88	0.54
2:B:18:VAL:HG22	2:B:86:LEU:CD2	2.28	0.54
1:A:204:GLN:HB3	3:A:264:HOH:O	2.07	0.54
2:H:114:THR:HG22	3:H:234:HOH:O	2.08	0.54
2:H:1:GLN:CB	2:H:3:GLN:HG3	2.39	0.53
1:L:123:PHE:HZ	2:H:143:ALA:HB1	1.71	0.53
2:B:125:PRO:HB3	2:B:151:TYR:HB3	1.90	0.53
2:B:169:VAL:CG2	2:B:188:VAL:HG13	2.39	0.53
2:H:1:GLN:C	2:H:3:GLN:N	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:HD3	1:A:67:PHE:O	2.08	0.53
2:H:100:GLU:OE2	2:H:102:LEU:HB2	2.08	0.52
1:A:42:LEU:HD13	1:A:91:TYR:CZ	2.44	0.52
2:H:1:GLN:C	2:H:3:GLN:H	2.11	0.52
2:B:190:VAL:HB	2:B:191:PRO:HD2	1.91	0.52
1:L:2:LEU:HD13	1:L:98:HIS:CD2	2.45	0.52
1:L:43:GLN:HE22	2:H:39:GLN:HE22	1.58	0.52
1:L:66:ARG:NH1	1:L:87:ASP:OD1	2.43	0.52
2:H:190:VAL:HB	2:H:191:PRO:HD2	1.93	0.51
1:A:148:GLU:HA	3:A:224:HOH:O	2.09	0.51
2:H:52:ASN:HD22	2:H:54:TYR:N	2.05	0.51
1:L:198:ALA:CB	1:L:213:SER:HB3	2.41	0.51
1:A:179:SER:HB2	2:B:170:HIS:HD2	1.75	0.51
1:A:202:THR:HB	1:A:209:PRO:HG3	1.92	0.51
2:H:134:SER:C	2:H:136:SER:H	2.14	0.51
1:L:28:SER:HA	1:L:74:THR:HG22	1.93	0.51
1:L:202:THR:HB	1:L:209:PRO:HG3	1.91	0.51
1:L:126:SER:OG	1:L:128:GLU:HG2	2.10	0.51
2:B:161:ASN:HD21	2:B:200:TYR:HA	1.76	0.50
1:L:2:LEU:HD21	1:L:29:LEU:HD21	1.92	0.50
2:B:3:GLN:HA	2:B:108:TYR:CZ	2.45	0.50
1:A:216:ARG:HB2	1:A:216:ARG:CZ	2.41	0.50
1:L:12:PRO:HB2	1:L:112:LYS:HB2	1.94	0.50
1:A:31:HIS:CE1	2:B:104:ARG:HH22	2.30	0.50
2:B:26:GLY:C	2:B:28:THR:H	2.12	0.50
1:L:66:ARG:NH1	1:L:84:GLU:HG3	2.27	0.50
2:H:2:VAL:HB	2:H:108:TYR:CD2	2.46	0.50
1:A:124:PRO:HB3	1:A:214:PHE:CZ	2.47	0.50
2:B:52:ASN:HD22	2:B:54:TYR:N	2.08	0.49
1:L:150:LYS:HE3	1:L:152:GLN:HG3	1.94	0.49
1:L:59:ARG:HD3	1:L:67:PHE:O	2.12	0.49
1:A:203:HIS:CD2	1:A:205:GLY:N	2.78	0.49
1:A:25:SER:HB2	1:A:29:LEU:HD21	1.94	0.49
1:A:95:GLN:NE2	1:A:102:THR:OG1	2.46	0.49
2:H:130:LEU:HB2	2:H:145:GLY:C	2.33	0.49
1:L:147:ARG:HH11	1:L:168:VAL:HG11	1.78	0.49
1:L:37:TYR:CE2	2:H:104:ARG:HD3	2.48	0.49
1:L:39:HIS:HD2	1:L:54:TYR:HA	1.78	0.48
1:L:39:HIS:NE2	2:H:105:THR:HG22	2.29	0.48
2:B:161:ASN:ND2	2:B:201:ILE:H	2.10	0.48
1:L:31:HIS:HB3	1:L:33:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLN:HG2	1:A:176:SER:HA	1.96	0.48
1:L:113:ARG:HD3	1:L:114:THR:O	2.14	0.48
1:A:39:HIS:HD2	1:A:54:TYR:HA	1.79	0.47
2:B:148:VAL:HG22	2:B:148:VAL:O	2.14	0.47
1:L:147:ARG:NH1	3:L:230:HOH:O	2.46	0.47
1:L:40:TRP:CZ3	1:L:93:CYS:HB3	2.50	0.47
2:H:169:VAL:HG22	2:H:188:VAL:HG13	1.97	0.47
1:L:31:HIS:CD2	1:L:33:ASN:H	2.31	0.47
1:A:31:HIS:HB3	1:A:33:ASN:OD1	2.14	0.47
1:A:91:TYR:O	1:A:106:GLY:HA2	2.15	0.47
1:L:113:ARG:HD2	1:L:145:TYR:CG	2.50	0.47
1:L:141:LEU:HD11	1:L:201:VAL:CG2	2.44	0.47
2:H:190:VAL:HB	2:H:191:PRO:CD	2.45	0.47
1:A:131:LYS:HB2	1:A:131:LYS:HE3	1.60	0.47
1:A:99:VAL:CB	1:A:100:PRO:CD	2.88	0.47
1:L:31:HIS:HE1	2:H:104:ARG:HH22	1.62	0.47
1:L:200:GLU:HG3	1:L:211:THR:HG22	1.96	0.47
1:A:39:HIS:HD2	1:A:54:TYR:HB2	1.80	0.46
1:L:171:GLN:HG2	1:L:176:SER:HA	1.97	0.46
1:A:66:ARG:CZ	1:A:84:GLU:HG3	2.44	0.46
1:A:198:ALA:HB2	1:A:213:SER:HB3	1.95	0.46
1:A:110:GLU:OE1	1:A:178:TYR:OH	2.33	0.46
2:H:52:ASN:ND2	2:H:55:THR:H	2.13	0.46
2:B:103:ARG:O	2:B:104:ARG:HB2	2.14	0.46
1:L:130:LEU:HD21	1:L:191:TYR:CD2	2.50	0.46
2:H:20:ILE:HD11	2:H:115:VAL:CG2	2.46	0.46
1:A:100:PRO:O	1:A:102:THR:HG23	2.16	0.46
1:A:31:HIS:CD2	1:A:33:ASN:H	2.28	0.46
2:H:161:ASN:ND2	2:H:201:ILE:H	2.14	0.46
1:L:195:LYS:O	1:L:215:ASN:O	2.34	0.45
1:A:25:SER:CB	1:A:29:LEU:HD21	2.46	0.45
1:L:23:CYS:HB2	1:L:40:TRP:CH2	2.52	0.45
1:L:198:ALA:HB2	1:L:213:SER:CB	2.46	0.45
1:L:49:PRO:HD2	2:H:109:TRP:CE3	2.51	0.45
1:L:31:HIS:CE1	2:H:104:ARG:HH22	2.33	0.45
2:H:103:ARG:NH1	2:H:103:ARG:HG3	2.32	0.45
1:A:4:MET:HB3	1:A:4:MET:HE2	1.78	0.45
1:A:130:LEU:HD21	1:A:191:TYR:CD2	2.52	0.45
1:L:35:ASN:OD1	1:L:35:ASN:N	2.49	0.45
2:B:169:VAL:C	2:B:170:HIS:HD1	2.19	0.45
1:A:123:PHE:CE2	2:B:143:ALA:HB1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:29:LEU:HD13	1:L:95:GLN:HB2	1.98	0.44
2:H:191:PRO:HD2	2:H:194:SER:OG	2.18	0.44
2:H:1:GLN:O	2:H:3:GLN:N	2.51	0.44
1:A:206:LEU:HD22	1:A:210:VAL:CG2	2.48	0.44
1:A:206:LEU:HD22	1:A:210:VAL:HG21	1.99	0.44
1:A:2:LEU:HD21	1:A:29:LEU:CD2	2.47	0.44
1:A:66:ARG:NH1	1:A:87:ASP:OD1	2.51	0.44
1:A:2:LEU:HD22	1:A:95:GLN:CG	2.48	0.44
1:L:39:HIS:CD2	1:L:55:LYS:H	2.35	0.44
2:B:62:ASP:OD1	2:B:65:LYS:NZ	2.51	0.44
2:H:35:ASN:HD22	2:H:35:ASN:N	2.16	0.44
1:A:202:THR:HG22	1:A:209:PRO:HB3	1.99	0.43
1:L:118:PRO:HD3	1:L:203:HIS:CD2	2.52	0.43
2:B:3:GLN:HA	2:B:108:TYR:OH	2.18	0.43
1:L:39:HIS:HD2	1:L:54:TYR:CA	2.32	0.43
2:H:25:SER:O	2:H:26:GLY:O	2.36	0.43
1:L:117:ALA:HB1	1:L:206:LEU:HD23	2.00	0.43
2:B:40:ALA:HB3	2:B:43:LYS:HB2	2.00	0.43
2:H:100:GLU:OE1	2:H:103:ARG:HB2	2.18	0.43
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.54	0.43
1:A:95:GLN:HG2	1:A:97:THR:H	1.84	0.43
2:H:28:THR:HG22	3:H:275:HOH:O	2.18	0.43
2:H:114:THR:CG2	3:H:234:HOH:O	2.64	0.43
1:A:141:LEU:HD21	1:A:201:VAL:HG13	2.00	0.43
1:A:71:GLY:HA3	1:A:76:PHE:CD2	2.53	0.43
2:H:158:VAL:HA	2:H:203:ASN:O	2.19	0.43
1:A:54:TYR:HD1	1:A:55:LYS:HG3	1.82	0.43
2:B:130:LEU:HB2	2:B:145:GLY:C	2.39	0.43
1:A:124:PRO:HB3	1:A:214:PHE:CE1	2.54	0.43
1:A:113:ARG:HD2	1:A:145:TYR:CB	2.49	0.42
1:A:42:LEU:HD13	1:A:91:TYR:CE1	2.54	0.42
1:A:35:ASN:N	1:A:35:ASN:OD1	2.51	0.42
2:B:18:VAL:O	2:B:82:GLN:HA	2.18	0.42
1:L:62:GLY:HA3	3:L:253:HOH:O	2.19	0.42
1:L:95:GLN:HG2	1:L:97:THR:H	1.84	0.42
2:B:174:ALA:HA	2:B:184:LEU:HB3	2.01	0.42
1:A:81:SER:O	1:A:82:ARG:O	2.38	0.42
1:A:147:ARG:HH11	1:A:168:VAL:HG11	1.83	0.42
2:B:73:GLU:HB2	2:B:80:TYR:CE1	2.49	0.42
2:B:4:LEU:N	2:B:108:TYR:CE1	2.88	0.42
1:L:123:PHE:HA	1:L:124:PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:NE2	1:A:19:ALA:O	2.52	0.42
2:H:161:ASN:HD21	2:H:200:TYR:HA	1.85	0.41
1:L:47:GLN:HB3	3:L:224:HOH:O	2.20	0.41
2:H:162:SER:H	2:H:203:ASN:ND2	2.07	0.41
1:L:39:HIS:HD2	1:L:54:TYR:HB2	1.85	0.41
1:A:179:SER:OG	2:B:170:HIS:CD2	2.73	0.41
2:B:23:LYS:HD2	2:B:78:THR:OG1	2.20	0.41
2:B:149:LYS:HG3	2:B:150:ASP:CG	2.40	0.41
1:A:29:LEU:HD13	1:A:95:GLN:HB2	2.03	0.41
1:A:215:ASN:O	1:A:216:ARG:C	2.59	0.41
2:H:26:GLY:O	2:H:27:TYR:C	2.59	0.41
2:H:28:THR:CG2	3:H:275:HOH:O	2.68	0.41
1:A:150:LYS:HE3	1:A:152:GLN:HG3	2.01	0.41
1:L:39:HIS:CD2	1:L:54:TYR:HA	2.56	0.41
2:H:18:VAL:O	2:H:82:GLN:HA	2.20	0.41
1:A:39:HIS:HD2	1:A:54:TYR:CA	2.33	0.41
1:A:39:HIS:CD2	1:A:54:TYR:HA	2.55	0.41
2:B:1:GLN:C	2:B:2:VAL:HG23	2.40	0.41
1:L:131:LYS:HE3	1:L:131:LYS:HB2	1.73	0.41
2:H:4:LEU:HA	2:H:4:LEU:HD23	1.84	0.41
2:H:103:ARG:HB3	2:H:105:THR:HG23	2.01	0.41
2:H:176:LEU:HD12	2:H:176:LEU:HA	1.78	0.41
1:A:44:LYS:NZ	3:A:249:HOH:O	2.48	0.41
1:A:192:GLU:HA	1:A:217:GLY:O	2.20	0.41
2:B:184:LEU:HD12	2:B:184:LEU:C	2.41	0.40
1:L:54:TYR:CD1	2:H:103:ARG:HD2	2.56	0.40
1:L:196:VAL:HG13	1:L:215:ASN:HB3	2.03	0.40
1:L:141:LEU:HD11	1:L:201:VAL:HG22	2.04	0.40
1:A:147:ARG:NH1	1:A:168:VAL:HG11	2.37	0.40
2:B:8:GLY:O	2:B:113:THR:HG23	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:GLU:OE2	2:B:89:GLU:OE2[2_556]	1.99	0.21
2:H:89:GLU:OE2	2:H:89:GLU:OE2[2_555]	2.10	0.10

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	A	215/217 (99%)	196 (91%)	15 (7%)	4 (2%)	10 4
1	L	215/217 (99%)	197 (92%)	15 (7%)	3 (1%)	14 7
2	B	215/219 (98%)	197 (92%)	15 (7%)	3 (1%)	14 7
2	H	215/219 (98%)	194 (90%)	15 (7%)	6 (3%)	6 2
All	All	860/872 (99%)	784 (91%)	60 (7%)	16 (2%)	10 4

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	99	VAL
2	H	28	THR
1	A	99	VAL
1	A	216	ARG
2	B	2	VAL
1	L	82	ARG
1	L	216	ARG
2	H	26	GLY
2	H	27	TYR
2	H	143	ALA
1	A	82	ARG
2	B	143	ALA
1	A	73	GLY
2	B	3	GLN
2	H	2	VAL
2	H	144	LEU

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	A	193/193 (100%)	155 (80%)	38 (20%)	1 0
1	L	193/193 (100%)	157 (81%)	36 (19%)	2 1
2	B	183/185 (99%)	139 (76%)	44 (24%)	1 0
2	H	183/185 (99%)	143 (78%)	40 (22%)	1 0
All	All	752/756 (100%)	594 (79%)	158 (21%)	1 0

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLU
1	L	2	LEU
1	L	3	VAL
1	L	4	MET
1	L	9	LEU
1	L	11	LEU
1	L	18	GLN
1	L	20	SER
1	L	22	SER
1	L	35	ASN
1	L	50	LYS
1	L	55	LYS
1	L	61	SER
1	L	75	ASP
1	L	81	SER
1	L	84	GLU
1	L	95	GLN
1	L	108	LYS
1	L	113	ARG
1	L	114	THR
1	L	119	SER
1	L	128	GLU
1	L	134	THR
1	L	157	ASN
1	L	161	SER
1	L	167	SER
1	L	185	THR
1	L	186	LEU
1	L	193	LYS
1	L	195	LYS

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Mol	Chain	Res	Type
1	L	196	VAL
1	L	202	THR
1	L	204	GLN
1	L	207	SER
1	L	211	THR
1	L	216	ARG
2	H	1	GLN
2	H	2	VAL
2	H	5	LEU
2	H	11	LEU
2	H	18	VAL
2	H	23	LYS
2	H	27	TYR
2	H	28	THR
2	H	43	LYS
2	H	46	LYS
2	H	52	ASN
2	H	63	ASP
2	H	71	SER
2	H	73	GLU
2	H	74	THR
2	H	75	SER
2	H	77	SER
2	H	81	LEU
2	H	84	ASN
2	H	86	LEU
2	H	96	CYS
2	H	102	LEU
2	H	114	THR
2	H	138	SER
2	H	144	LEU
2	H	148	VAL
2	H	149	LYS
2	H	156	VAL
2	H	165	LEU
2	H	167	SER
2	H	181	LEU
2	H	188	VAL
2	H	189	THR
2	H	197	THR
2	H	199	THR
2	H	210	ASN

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Mol	Chain	Res	Type
2	H	212	LYS
2	H	213	VAL
2	H	215	LYS
2	H	216	LYS
1	A	1	GLU
1	A	2	LEU
1	A	3	VAL
1	A	4	MET
1	A	9	LEU
1	A	11	LEU
1	A	18	GLN
1	A	20	SER
1	A	22	SER
1	A	24	ARG
1	A	28	SER
1	A	35	ASN
1	A	55	LYS
1	A	61	SER
1	A	81	SER
1	A	84	GLU
1	A	95	GLN
1	A	108	LYS
1	A	113	ARG
1	A	114	THR
1	A	128	GLU
1	A	131	LYS
1	A	134	THR
1	A	147	ARG
1	A	157	ASN
1	A	161	SER
1	A	173	SER
1	A	174	LYS
1	A	185	THR
1	A	193	LYS
1	A	195	LYS
1	A	196	VAL
1	A	202	THR
1	A	204	GLN
1	A	207	SER
1	A	211	THR
1	A	213	SER
1	A	216	ARG

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Mol	Chain	Res	Type
2	B	2	VAL
2	B	3	GLN
2	B	5	LEU
2	B	11	LEU
2	B	12	LYS
2	B	18	VAL
2	B	25	SER
2	B	27	TYR
2	B	46	LYS
2	B	52	ASN
2	B	63	ASP
2	B	73	GLU
2	B	74	THR
2	B	75	SER
2	B	77	SER
2	B	81	LEU
2	B	84	ASN
2	B	86	LEU
2	B	96	CYS
2	B	101	ARG
2	B	102	LEU
2	B	114	THR
2	B	119	SER
2	B	133	SER
2	B	138	SER
2	B	144	LEU
2	B	148	VAL
2	B	149	LYS
2	B	156	VAL
2	B	165	LEU
2	B	167	SER
2	B	170	HIS
2	B	181	LEU
2	B	188	VAL
2	B	189	THR
2	B	192	SER
2	B	193	SER
2	B	197	THR
2	B	199	THR
2	B	210	ASN
2	B	212	LYS
2	B	213	VAL

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Mol	Chain	Res	Type
2	B	215	LYS
2	B	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	18	GLN
1	L	31	HIS
1	L	39	HIS
1	L	43	GLN
1	L	58	ASN
1	L	95	GLN
1	L	143	ASN
1	L	157	ASN
1	L	171	GLN
1	L	203	HIS
2	H	52	ASN
2	H	82	GLN
2	H	84	ASN
2	H	161	ASN
2	H	203	ASN
1	A	18	GLN
1	A	31	HIS
1	A	39	HIS
1	A	43	GLN
1	A	47	GLN
1	A	95	GLN
1	A	98	HIS
1	A	171	GLN
1	A	203	HIS
2	B	1	GLN
2	B	3	GLN
2	B	52	ASN
2	B	82	GLN
2	B	84	ASN
2	B	161	ASN
2	B	177	GLN
2	B	203	ASN
2	B	205	ASN

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	A	217/217 (100%)	0.78	25 (11%) 6 9	22, 37, 57, 83	0
1	L	217/217 (100%)	0.70	20 (9%) 11 15	22, 38, 55, 85	0
2	B	217/219 (99%)	0.83	23 (10%) 8 11	14, 30, 64, 99	0
2	H	217/219 (99%)	0.95	30 (13%) 4 5	15, 29, 65, 99	0
All	All	868/872 (99%)	0.82	98 (11%) 7 9	14, 33, 59, 99	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	2	VAL	14.2
2	B	134	SER	14.0
2	H	137	THR	13.7
2	H	139	GLY	11.6
2	B	137	THR	11.4
2	H	134	SER	10.8
2	B	138	SER	10.1
2	B	1	GLN	10.0
2	B	135	LYS	9.5
2	B	2	VAL	9.4
1	L	7	THR	8.4
2	H	135	LYS	8.2
2	B	139	GLY	7.8
2	H	1	GLN	7.8
2	H	138	SER	7.6
2	H	136	SER	7.4
1	A	99	VAL	6.3
1	L	99	VAL	6.2
1	A	7	THR	6.1
2	H	27	TYR	5.1
2	H	96	CYS	4.8

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Mol	Chain	Res	Type	RSRZ
2	H	108	TYR	4.7
1	A	2	LEU	4.7
2	B	26	GLY	4.5
2	B	27	TYR	4.4
2	B	96	CYS	4.4
1	L	45	PRO	4.3
2	H	54	TYR	4.1
1	A	38	LEU	4.1
2	B	108	TYR	4.0
2	H	101	ARG	3.7
2	B	101	ARG	3.7
2	H	102	LEU	3.6
2	B	3	GLN	3.5
2	H	26	GLY	3.5
2	H	42	GLY	3.5
1	A	45	PRO	3.4
1	A	1	GLU	3.4
1	A	209	PRO	3.3
1	L	196	VAL	3.2
2	H	197	THR	3.2
2	B	81	LEU	3.2
1	L	1	GLU	3.1
1	L	38	LEU	3.1
1	A	217	GLY	3.1
1	A	32	SER	3.0
1	L	81	SER	3.0
2	H	133	SER	3.0
1	L	78	LEU	3.0
2	B	102	LEU	2.9
2	B	36	TRP	2.9
2	B	136	SER	2.8
1	A	61	SER	2.8
2	H	143	ALA	2.8
1	A	46	GLY	2.8
1	A	78	LEU	2.7
2	B	97	VAL	2.7
1	L	32	SER	2.7
2	H	3	GLN	2.6
1	L	215	ASN	2.6
1	A	81	SER	2.6
2	H	140	GLY	2.6
1	L	40	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	75	SER	2.4
1	A	34	GLY	2.4
1	L	207	SER	2.4
1	A	199	CYS	2.4
2	H	81	LEU	2.4
1	L	159	LEU	2.4
1	A	207	SER	2.4
1	A	174	LYS	2.4
2	H	22	CYS	2.3
1	L	82	ARG	2.3
1	A	159	LEU	2.3
2	H	23	LYS	2.3
2	B	37	VAL	2.2
2	B	143	ALA	2.2
1	L	209	PRO	2.2
2	H	37	VAL	2.2
1	L	208	SER	2.2
1	A	140	LEU	2.2
2	B	188	VAL	2.2
1	L	80	ILE	2.2
2	H	201	ILE	2.2
2	H	202	CYS	2.2
2	H	142	ALA	2.2
1	A	24	ARG	2.1
1	A	208	SER	2.1
2	H	36	TRP	2.1
1	A	82	ARG	2.1
1	A	189	ALA	2.1
1	L	91	TYR	2.1
1	A	40	TRP	2.1
1	L	150	LYS	2.1
2	B	43	LYS	2.1
1	L	92	PHE	2.0
1	A	30	VAL	2.0
2	H	79	ALA	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

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.