



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:16 AM UTC

PDB ID : 5Y2K / pdb_00005y2k
Title : A human antibody AF4H1L1
Authors : Xiao, H.; Qi, J.; Gao, F.G.
Deposited on : 2017-07-26
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

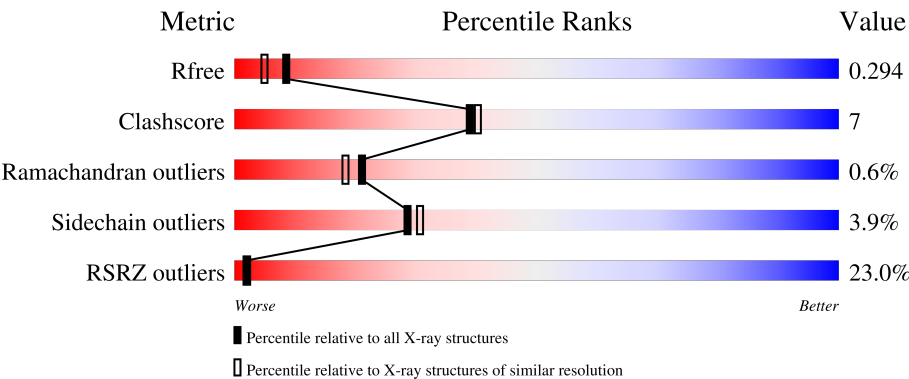
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.10 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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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 $\leq 5\%$. 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	A	233	
1	C	233	
1	E	233	
1	G	233	
2	B	218	

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Mol	Chain	Length	Quality of chain
2	D	218	40% 68% 21% 6% 5%
2	F	218	8% 81% 14% • 5%
2	H	218	43% 75% 19% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13469 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 a group 2 HA binding antibody AF4H1K1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1691	1076	285	324	6			
1	C	216	Total	C	N	O	S	0	0	0
			1626	1029	276	315	6			
1	E	223	Total	C	N	O	S	0	0	0
			1691	1076	285	324	6			
1	G	220	Total	C	N	O	S	0	0	0
			1658	1052	281	319	6			

- Molecule 2 is a protein called a group 2 HA binding antibody AF4H1K1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	1	0
			1564	978	257	323	6			
2	D	208	Total	C	N	O	S	0	0	0
			1558	975	256	321	6			
2	F	208	Total	C	N	O	S	0	0	0
			1558	975	256	321	6			
2	H	208	Total	C	N	O	S	0	0	0
			1558	975	256	321	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total	O	0	0
			110	110		
3	B	87	Total	O	0	0
			87	87		
3	C	47	Total	O	0	0
			47	47		
3	D	27	Total	O	0	0
			27	27		

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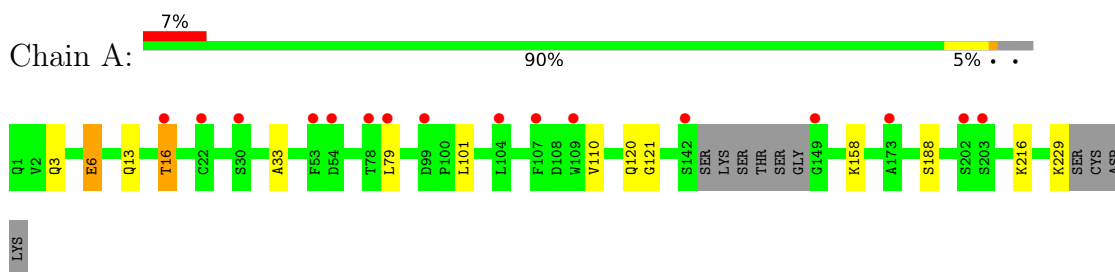
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	159	Total 159	O 159	0	0
3	F	91	Total 91	O 91	0	0
3	G	25	Total 25	O 25	0	0
3	H	19	Total 19	O 19	0	0

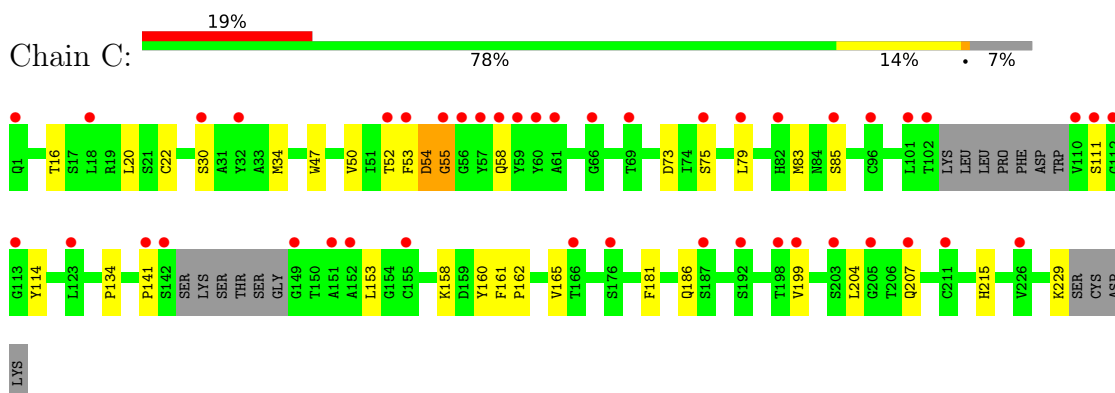
3 Residue-property plots

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.

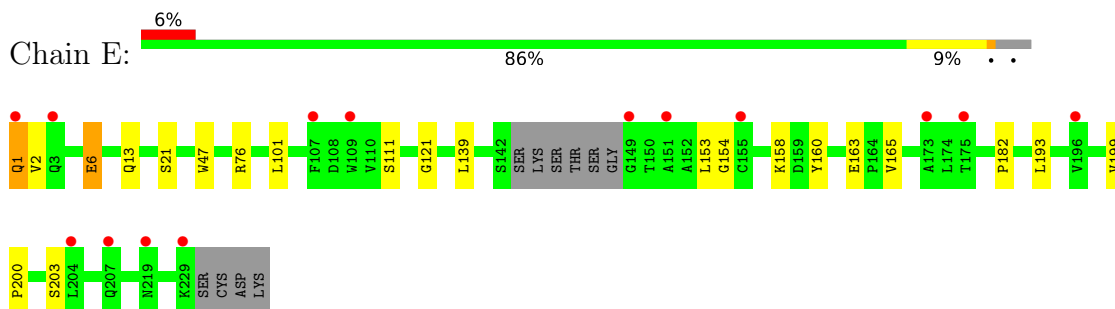
- Molecule 1: a group 2 HA binding antibody AF4H1K1 Fab heavy chain



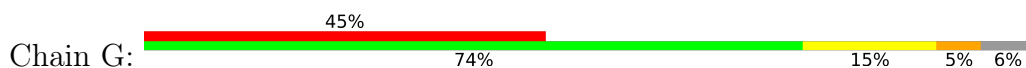
- Molecule 1: a group 2 HA binding antibody AF4H1K1 Fab heavy chain

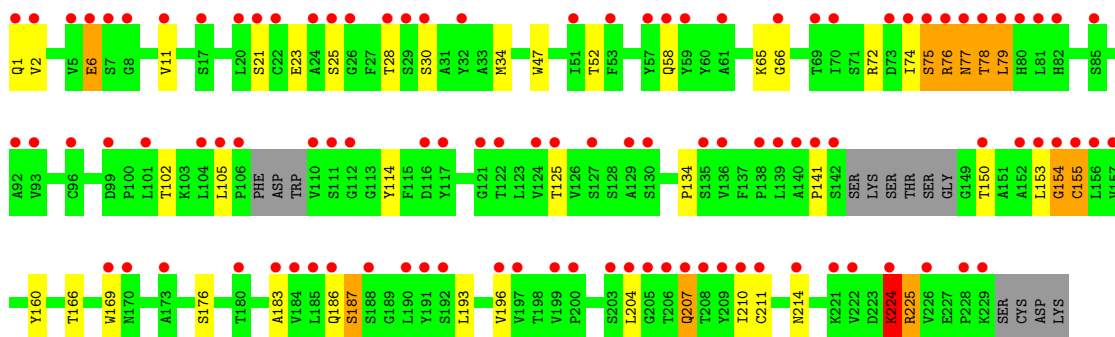


- Molecule 1: a group 2 HA binding antibody AF4H1K1 Fab heavy chain

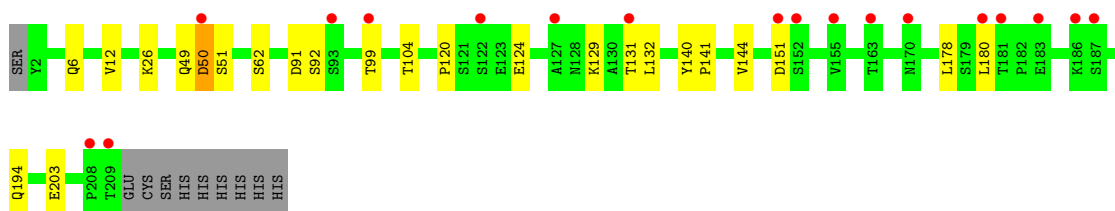
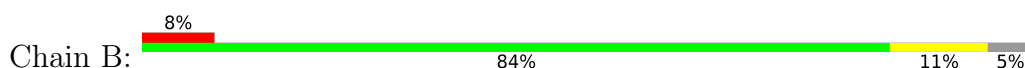


- Molecule 1: a group 2 HA binding antibody AF4H1K1 Fab heavy chain

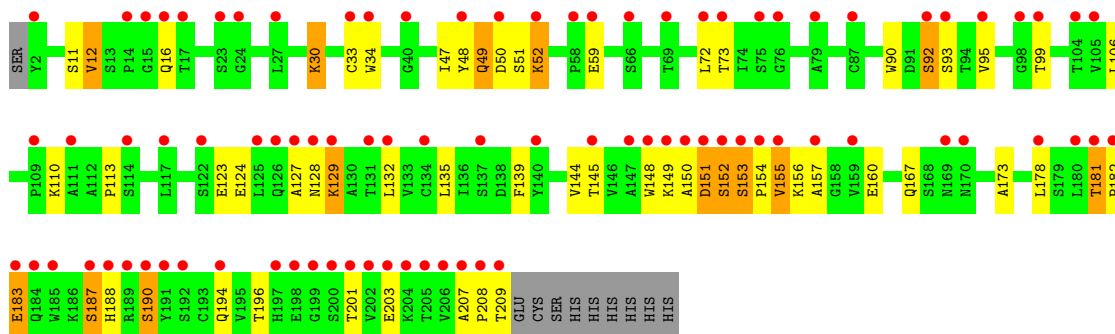
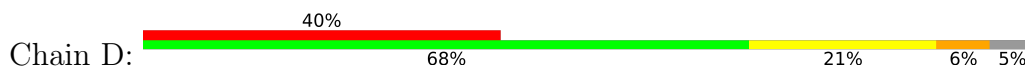




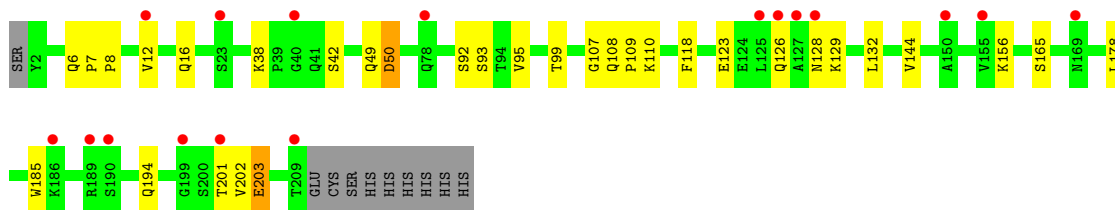
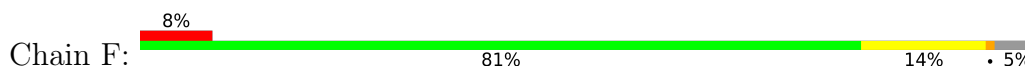
- Molecule 2: a group 2 HA binding antibody AF4H1K1 Fab light chain



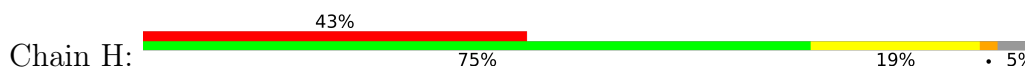
- Molecule 2: a group 2 HA binding antibody AF4H1K1 Fab light chain

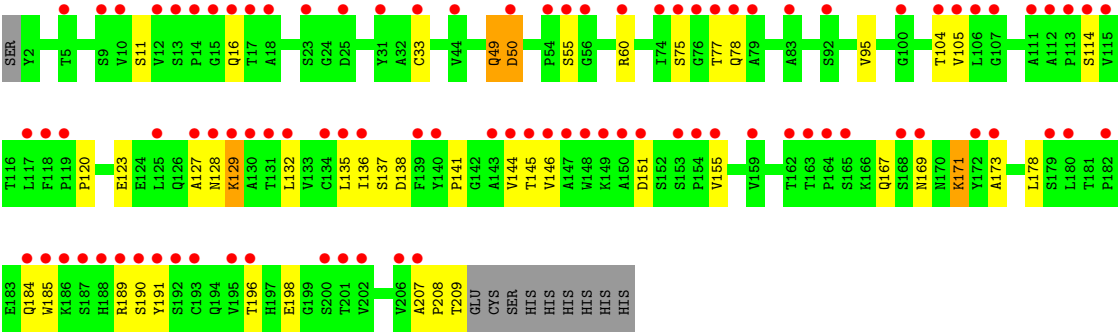


- Molecule 2: a group 2 HA binding antibody AF4H1K1 Fab light chain



- Molecule 2: a group 2 HA binding antibody AF4H1K1 Fab light chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.27Å 90.12Å 111.40Å 90.00° 102.38° 90.00°	Depositor
Resolution (Å)	41.63 – 2.10 41.63 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (41.63-2.10) 98.0 (41.63-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9-1692	Depositor
R, R_{free}	0.220 , 0.259 (Not available) , 0.294	Depositor DCC
R_{free} test set	5966 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13469	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.37	0/1736	0.71	0/2369
1	C	0.35	0/1666	0.78	2/2271 (0.1%)
1	E	0.37	0/1736	0.76	3/2369 (0.1%)
1	G	0.40	0/1699	0.91	5/2316 (0.2%)
2	B	0.37	0/1603	0.74	1/2192 (0.0%)
2	D	0.42	0/1597	0.89	5/2184 (0.2%)
2	F	0.42	0/1597	0.79	2/2184 (0.1%)
2	H	0.33	0/1597	0.76	3/2184 (0.1%)
All	All	0.38	0/13231	0.80	21/18069 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	76	ARG	N-CA-C	14.77	134.56	111.81
2	H	50	ASP	CB-CA-C	-7.19	96.11	110.42
2	D	153	SER	CA-C-N	7.14	128.76	119.84
2	D	153	SER	C-N-CA	7.14	128.76	119.84
1	G	75	SER	N-CA-C	-6.24	105.98	113.97
2	B	50	ASP	CB-CA-C	-6.22	98.03	110.42
2	D	151	ASP	N-CA-C	-6.20	97.61	110.80
1	C	111	SER	N-CA-C	6.06	119.12	110.10
1	C	55	GLY	N-CA-C	-5.96	99.06	113.18
2	F	50	ASP	CB-CA-C	-5.75	98.99	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	199	VAL	CA-C-N	-5.50	114.05	119.99
1	E	199	VAL	C-N-CA	-5.50	114.05	119.99
1	G	224	LYS	CG-CD-CE	-5.43	98.82	111.30
2	D	127	ALA	N-CA-C	-5.43	102.97	110.35
2	D	156	LYS	N-CA-C	-5.41	106.05	113.30
1	G	78	THR	N-CA-C	5.30	118.02	108.48
1	G	154	GLY	N-CA-C	5.25	118.24	110.42
2	H	50	ASP	N-CA-C	5.22	121.93	110.80
2	F	185	TRP	N-CA-C	5.15	117.30	111.02
2	H	49	GLN	N-CA-C	5.13	118.81	112.24
1	E	154	GLY	N-CA-C	5.07	118.54	111.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	54	ASP	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	A	1691	0	1648	10	0
1	C	1626	0	1582	22	0
1	E	1691	0	1648	14	0
1	G	1658	0	1623	45	0
2	B	1564	0	1508	17	0
2	D	1558	0	1504	39	0
2	F	1558	0	1504	17	0
2	H	1558	0	1504	24	0
3	A	110	0	0	3	0
3	B	87	0	0	6	1
3	C	47	0	0	0	0
3	D	27	0	0	0	0
3	E	159	0	0	5	1
3	F	91	0	0	3	0
3	G	25	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	19	0	0	1	0
All	All	13469	0	12521	173	1

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 7.

All (173) 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:G:76:ARG:O	1:G:78:THR:OG1	1.80	0.99
1:G:176:SER:OG	3:G:301:HOH:O	1.87	0.92
1:E:76:ARG:NH2	3:E:303:HOH:O	2.11	0.83
1:A:13:GLN:OE1	3:A:301:HOH:O	1.98	0.82
1:G:25:SER:HA	1:G:77:ASN:HD21	1.45	0.81
1:C:34:MET:HB3	1:C:79:LEU:HD21	1.62	0.80
1:G:211:CYS:SG	1:G:224:LYS:HE2	2.24	0.76
1:G:76:ARG:HB3	1:G:76:ARG:HH21	1.50	0.76
1:G:76:ARG:HB3	1:G:76:ARG:NH2	2.00	0.76
2:B:180:LEU:O	3:B:301:HOH:O	2.02	0.75
1:A:120:GLN:HG3	1:G:28:THR:HG21	1.68	0.74
1:E:111:SER:OG	3:E:302:HOH:O	2.06	0.74
2:H:132:LEU:HD12	2:H:178:LEU:HD23	1.69	0.74
2:D:92:SER:OG	2:D:93:SER:N	2.18	0.72
2:D:151:ASP:OD1	2:D:190:SER:OG	2.04	0.72
1:E:1:GLN:OE1	1:E:2:VAL:N	2.20	0.71
2:D:49:GLN:O	2:D:50:ASP:HB2	1.90	0.71
1:G:224:LYS:HG2	1:G:224:LYS:O	1.92	0.69
2:D:148:TRP:O	2:D:155:VAL:HG22	1.92	0.69
2:D:151:ASP:O	2:D:152:SER:HB2	1.94	0.68
1:G:76:ARG:O	1:G:77:ASN:C	2.35	0.67
1:G:141:PRO:HG3	1:G:204:LEU:HD22	1.75	0.67
1:G:155:CYS:HA	1:G:224:LYS:HZ3	1.59	0.67
1:G:28:THR:HG22	1:G:30:SER:H	1.59	0.67
2:B:6:GLN:H	2:B:99:THR:HG22	1.60	0.67
1:G:25:SER:HA	1:G:77:ASN:ND2	2.10	0.66
1:G:196:VAL:HG11	2:H:135:LEU:HD13	1.77	0.65
2:D:187:SER:OG	2:D:188:HIS:N	2.28	0.64
2:D:148:TRP:O	2:D:149:LYS:HD3	1.97	0.64
1:G:155:CYS:CA	1:G:224:LYS:HZ3	2.10	0.64
2:H:11:SER:OG	2:H:198:GLU:OE2	2.13	0.63
2:D:30:LYS:HE2	2:D:90:TRP:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:VAL:HG13	2:D:16:GLN:HB3	1.81	0.62
2:H:127:ALA:O	2:H:129:LYS:N	2.32	0.62
2:D:150:ALA:O	2:D:190:SER:O	2.17	0.62
2:F:132:LEU:HD12	2:F:178:LEU:HD23	1.81	0.62
2:F:123:GLU:O	2:F:126:GLN:HB2	2.01	0.61
2:D:145:THR:HB	2:D:196:THR:HB	1.81	0.61
1:G:134:PRO:HB3	1:G:160:TYR:HB3	1.83	0.60
1:C:34:MET:CB	1:C:79:LEU:HD21	2.31	0.60
2:D:132:LEU:HD12	2:D:178:LEU:HD23	1.84	0.59
2:B:131:THR:HG22	3:B:362:HOH:O	2.02	0.59
2:B:132:LEU:HD12	2:B:178:LEU:HD23	1.85	0.58
2:D:128:ASN:C	2:D:129:LYS:HD2	2.28	0.58
1:G:52:THR:HG22	1:G:105:LEU:HD13	1.85	0.58
1:G:23:GLU:HA	1:G:77:ASN:O	2.04	0.57
2:B:49:GLN:OE1	3:B:303:HOH:O	2.18	0.57
2:D:129:LYS:HD2	2:D:129:LYS:N	2.20	0.56
1:C:85:SER:O	1:C:85:SER:OG	2.21	0.56
2:H:49:GLN:O	2:H:50:ASP:HB2	2.04	0.56
1:G:154:GLY:O	1:G:224:LYS:NZ	2.38	0.56
2:D:194:GLN:NE2	2:D:203:GLU:OE1	2.38	0.56
1:C:158:LYS:NZ	2:D:124:GLU:OE1	2.37	0.55
1:E:13:GLN:NE2	3:E:310:HOH:O	2.39	0.55
2:B:124:GLU:OE1	2:B:131:THR:HG23	2.06	0.55
2:D:194:GLN:HG2	2:D:201:THR:CG2	2.37	0.55
2:D:181:THR:HB	2:D:183:GLU:HG2	1.89	0.55
1:G:65:LYS:HD2	1:G:66:GLY:N	2.22	0.54
2:D:49:GLN:O	2:D:50:ASP:CB	2.55	0.54
2:B:62:SER:OG	3:B:304:HOH:O	2.18	0.54
1:G:72:ARG:N	3:G:306:HOH:O	2.39	0.54
2:B:194:GLN:HG2	2:B:203:GLU:HB2	1.90	0.54
2:F:12:VAL:HG13	2:F:16:GLN:HB2	1.90	0.54
1:G:141:PRO:O	3:G:302:HOH:O	2.19	0.53
1:C:165:VAL:HG22	1:C:215:HIS:CD2	2.43	0.53
1:C:186:GLN:HG2	2:D:160:GLU:HG2	1.91	0.53
1:A:188:SER:N	3:A:302:HOH:O	2.42	0.52
1:E:200:PRO:O	1:E:203:SER:OG	2.27	0.52
1:G:207:GLN:HG3	3:G:314:HOH:O	2.08	0.52
1:A:3:GLN:HE22	1:G:75:SER:HA	1.75	0.51
2:F:107:GLY:O	3:F:301:HOH:O	2.18	0.51
1:C:58:GLN:CD	1:C:58:GLN:H	2.19	0.51
1:G:47:TRP:CG	2:H:95:VAL:HB	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:PRO:HD3	2:H:132:LEU:HD23	1.93	0.50
1:G:1:GLN:N	3:G:309:HOH:O	2.45	0.50
2:H:114:SER:OG	2:H:137:SER:HB2	2.12	0.50
1:G:76:ARG:NH2	1:G:76:ARG:CB	2.73	0.49
1:C:199:VAL:HG21	1:C:204:LEU:HD21	1.94	0.49
1:G:210:ILE:HG12	1:G:225:ARG:HB2	1.94	0.49
2:F:99:THR:HG23	3:F:316:HOH:O	2.13	0.48
2:H:16:GLN:O	2:H:77:THR:HG22	2.13	0.48
1:C:52:THR:OG1	1:C:55:GLY:O	2.31	0.48
1:G:34:MET:CB	1:G:79:LEU:HD21	2.43	0.48
1:E:47:TRP:CG	2:F:95:VAL:HB	2.48	0.48
1:G:74:ILE:HG22	1:G:74:ILE:O	2.13	0.48
1:A:13:GLN:O	1:A:16:THR:HB	2.14	0.48
2:D:59:GLU:OE1	2:D:59:GLU:N	2.45	0.48
1:G:183:ALA:HA	1:G:193:LEU:HB3	1.96	0.48
1:E:165:VAL:HG22	1:E:193:LEU:HD21	1.96	0.48
2:H:151:ASP:OD1	2:H:189:ARG:HG2	2.13	0.48
2:B:49:GLN:O	2:B:50:ASP:HB2	2.13	0.47
2:D:151:ASP:OD1	2:D:190:SER:CB	2.62	0.47
1:E:160:TYR:CE2	1:E:165:VAL:HG13	2.49	0.47
1:A:6:GLU:CD	1:A:121:GLY:H	2.22	0.47
2:D:48:TYR:O	2:D:49:GLN:CB	2.58	0.47
2:D:183:GLU:CD	2:D:183:GLU:H	2.21	0.47
1:G:102:THR:CG2	1:G:105:LEU:HD11	2.44	0.47
2:H:138:ASP:HA	2:H:171:LYS:HD2	1.96	0.47
2:B:91:ASP:O	2:B:92:SER:OG	2.30	0.47
2:D:11:SER:HB2	2:D:106:LEU:HD21	1.96	0.47
2:H:185:TRP:CH2	2:H:208:PRO:HA	2.50	0.47
1:C:165:VAL:HG22	1:C:215:HIS:HD2	1.79	0.46
1:G:186:GLN:CD	1:G:187:SER:H	2.21	0.46
2:F:38:LYS:NZ	3:F:310:HOH:O	2.47	0.46
1:G:58:GLN:N	1:G:58:GLN:OE1	2.49	0.46
1:G:186:GLN:OE1	1:G:187:SER:N	2.36	0.46
1:C:114:TYR:HB3	2:D:33:CYS:SG	2.56	0.46
1:C:20:LEU:HG	1:C:83:MET:HE2	1.97	0.46
2:H:104:THR:HG21	2:H:141:PRO:HB3	1.96	0.46
1:C:73:ASP:OD1	1:C:75:SER:HB3	2.16	0.45
1:C:141:PRO:HB3	1:C:153:LEU:HB3	1.98	0.45
2:H:167:GLN:OE1	2:H:173:ALA:HB2	2.17	0.45
2:D:128:ASN:O	2:D:129:LYS:HD2	2.17	0.45
2:H:114:SER:OG	2:H:137:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:PHE:CZ	2:D:135:LEU:HB3	2.51	0.45
1:E:158:LYS:NZ	3:E:319:HOH:O	2.50	0.45
1:G:6:GLU:H	1:G:6:GLU:HG2	1.65	0.45
2:D:123:GLU:OE1	2:D:123:GLU:N	2.40	0.45
1:G:11:VAL:HG22	1:G:125:THR:HB	1.98	0.45
1:G:65:LYS:HD2	3:G:304:HOH:O	2.17	0.44
2:H:189:ARG:HG3	2:H:190:SER:N	2.33	0.44
1:C:47:TRP:CG	2:D:95:VAL:HB	2.52	0.44
1:G:25:SER:CA	1:G:77:ASN:HD21	2.25	0.44
2:B:120:PRO:HD3	2:B:132:LEU:HD23	2.00	0.44
2:B:151:ASP:HB2	3:B:306:HOH:O	2.17	0.44
2:D:181:THR:HG22	2:D:182:PRO:HD2	1.99	0.44
2:F:92:SER:OG	2:F:93:SER:N	2.39	0.44
2:H:55:SER:O	3:H:302:HOH:O	2.21	0.44
2:D:34:TRP:CD2	2:D:72:LEU:HB2	2.53	0.43
2:F:194:GLN:HG2	2:F:203:GLU:HB2	2.00	0.43
2:H:184:GLN:O	2:H:191:TYR:OH	2.32	0.43
1:A:216:LYS:HE3	1:A:216:LYS:HB2	1.91	0.43
2:F:49:GLN:O	2:F:50:ASP:HB2	2.18	0.43
1:C:22:CYS:HB3	1:C:79:LEU:HB2	2.00	0.43
1:C:134:PRO:HB3	1:C:160:TYR:HB3	2.00	0.43
2:F:7:PRO:HA	2:F:8:PRO:HD3	1.84	0.43
1:G:76:ARG:CB	1:G:76:ARG:CZ	2.96	0.43
2:D:34:TRP:HB2	2:D:47:ILE:HB	2.00	0.43
2:D:194:GLN:HG3	2:D:203:GLU:CB	2.48	0.43
2:D:48:TYR:CE2	2:D:52:LYS:HE2	2.54	0.42
2:F:108:GLN:HB2	2:F:109:PRO:HD2	2.02	0.42
1:E:6:GLU:HA	1:E:21:SER:O	2.18	0.42
1:E:163:GLU:OE2	3:E:304:HOH:O	2.21	0.42
1:C:30:SER:O	1:C:53:PHE:HB2	2.20	0.42
2:H:78:GLN:O	2:H:105:VAL:HG21	2.19	0.42
1:C:34:MET:HG3	1:C:79:LEU:HD11	2.01	0.42
2:D:207:ALA:C	2:D:209:THR:H	2.27	0.42
1:A:158:LYS:NZ	2:B:131:THR:HG21	2.36	0.41
1:C:47:TRP:HZ2	1:C:50:VAL:HG12	1.84	0.41
1:E:139:LEU:HB3	2:F:118:PHE:CD1	2.55	0.41
2:B:104:THR:HG21	2:B:141:PRO:HB3	2.03	0.41
2:F:6:GLN:H	2:F:99:THR:HG22	1.85	0.41
2:H:132:LEU:HB2	2:H:178:LEU:HB3	2.01	0.41
1:A:3:GLN:OE1	1:G:75:SER:HB3	2.21	0.41
2:B:203:GLU:OE2	3:B:305:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:GLU:CD	1:E:121:GLY:H	2.28	0.41
1:E:182:PRO:HG2	2:F:165:SER:OG	2.20	0.41
1:G:114:TYR:HB3	2:H:33:CYS:SG	2.59	0.41
2:D:113:PRO:HB3	2:D:139:PHE:HB3	2.02	0.41
2:H:60:ARG:HB2	2:H:75:SER:O	2.21	0.41
2:F:128:ASN:O	2:F:129:LYS:HD3	2.20	0.41
2:H:207:ALA:C	2:H:209:THR:H	2.29	0.41
2:B:140:TYR:HA	2:B:141:PRO:C	2.46	0.41
2:H:169:ASN:ND2	2:H:171:LYS:HE2	2.35	0.41
2:B:124:GLU:HG2	2:B:129:LYS:O	2.21	0.41
1:C:161:PHE:HA	1:C:162:PRO:HA	1.88	0.41
1:G:166:THR:OG1	1:G:214:ASN:HB3	2.21	0.41
2:D:207:ALA:O	2:D:209:THR:N	2.47	0.41
1:A:33:ALA:HB2	3:A:327:HOH:O	2.21	0.40
2:D:167:GLN:OE1	2:D:173:ALA:HB2	2.21	0.40
1:G:6:GLU:HA	1:G:21:SER:O	2.20	0.40
1:G:169:TRP:CH2	1:G:211:CYS:HB3	2.57	0.40
2:F:132:LEU:HB2	2:F:178:LEU:HB3	2.03	0.40

All (1) 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)
3:B:384:HOH:O	3:E:375:HOH:O[2_7511]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/233 (84%)	191 (98%)	4 (2%)	0	100	100
1	C	210/233 (90%)	206 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	219/233 (94%)	216 (99%)	3 (1%)	0	100	100
1	G	214/233 (92%)	202 (94%)	11 (5%)	1 (0%)	24	22
2	B	207/218 (95%)	201 (97%)	5 (2%)	1 (0%)	24	22
2	D	206/218 (94%)	189 (92%)	10 (5%)	7 (3%)	3	1
2	F	206/218 (94%)	199 (97%)	7 (3%)	0	100	100
2	H	206/218 (94%)	198 (96%)	7 (3%)	1 (0%)	24	22
All	All	1663/1804 (92%)	1602 (96%)	51 (3%)	10 (1%)	21	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	153	SER
2	D	152	SER
2	D	187	SER
2	H	128	ASN
2	D	51	SER
2	B	51	SER
2	D	157	ALA
1	G	77	ASN
2	D	154	PRO
2	D	208	PRO

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	187/196 (95%)	181 (97%)	6 (3%)	34	38
1	C	180/196 (92%)	176 (98%)	4 (2%)	45	53
1	E	187/196 (95%)	183 (98%)	4 (2%)	47	54
1	G	184/196 (94%)	174 (95%)	10 (5%)	20	18
2	B	178/187 (95%)	175 (98%)	3 (2%)	53	62
2	D	177/187 (95%)	163 (92%)	14 (8%)	11	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	177/187 (95%)	170 (96%)	7 (4%)	28	29
2	H	177/187 (95%)	168 (95%)	9 (5%)	21	21
All	All	1447/1532 (94%)	1390 (96%)	57 (4%)	28	31

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	16	THR
1	A	79	LEU
1	A	101	LEU
1	A	110	VAL
1	A	229	LYS
2	B	12	VAL
2	B	26	LYS
2	B	144	VAL
1	C	16	THR
1	C	54	ASP
1	C	207	GLN
1	C	229	LYS
2	D	12	VAL
2	D	30	LYS
2	D	49	GLN
2	D	52	LYS
2	D	73	THR
2	D	92	SER
2	D	99	THR
2	D	110	LYS
2	D	129	LYS
2	D	144	VAL
2	D	155	VAL
2	D	181	THR
2	D	183	GLU
2	D	190	SER
1	E	1	GLN
1	E	6	GLU
1	E	101	LEU
1	E	153	LEU
2	F	42	SER
2	F	110	LYS
2	F	144	VAL

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Mol	Chain	Res	Type
2	F	156	LYS
2	F	201	THR
2	F	202	VAL
2	F	203	GLU
1	G	2	VAL
1	G	6	GLU
1	G	79	LEU
1	G	150	THR
1	G	153	LEU
1	G	155	CYS
1	G	187	SER
1	G	207	GLN
1	G	224	LYS
1	G	225	ARG
2	H	123	GLU
2	H	129	LYS
2	H	136	ILE
2	H	144	VAL
2	H	145	THR
2	H	146	VAL
2	H	155	VAL
2	H	171	LYS
2	H	196	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
2	B	37	GLN
2	B	68	ASN
2	B	78	GLN
1	C	39	GLN
2	D	37	GLN
2	D	49	GLN
2	D	126	GLN
2	D	194	GLN
2	D	197	HIS
1	E	13	GLN
2	F	49	GLN
2	F	65	ASN
1	G	120	GLN
2	H	188	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 oligosaccharides 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	A	223/233 (95%)	0.71	16 (7%)	21 23	34, 46, 62, 90	0
1	C	216/233 (92%)	1.26	44 (20%)	3 3	36, 54, 89, 119	0
1	E	223/233 (95%)	0.56	14 (6%)	26 27	29, 42, 79, 121	0
1	G	220/233 (94%)	2.11	104 (47%)	0 0	50, 70, 104, 142	0
2	B	208/218 (95%)	0.83	18 (8%)	16 16	17, 47, 70, 100	1 (0%)
2	D	208/218 (95%)	1.90	87 (41%)	0 1	41, 66, 128, 145	0
2	F	208/218 (95%)	0.69	17 (8%)	17 18	30, 46, 71, 125	0
2	H	208/218 (95%)	1.96	94 (45%)	0 1	46, 78, 112, 126	0
All	All	1714/1804 (95%)	1.25	394 (22%)	2 2	17, 55, 99, 145	1 (0%)

All (394) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	150	ALA	9.7
1	G	77	ASN	9.0
1	C	102	THR	9.0
2	D	185	TRP	6.8
1	C	110	VAL	6.5
1	G	74	ILE	6.3
1	G	155	CYS	6.2
1	G	82	HIS	6.2
2	D	76	GLY	5.6
2	H	12	VAL	5.3
2	H	196	THR	5.3
1	G	211	CYS	5.3
2	H	165	SER	5.1
1	G	153	LEU	5.1
1	G	196	VAL	4.9
2	D	125	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	G	57	TYR	4.8
1	G	184	VAL	4.7
1	G	226	VAL	4.4
1	G	204	LEU	4.4
1	G	210	ILE	4.4
1	C	142	SER	4.4
1	G	207	GLN	4.3
2	H	190	SER	4.3
1	G	197	VAL	4.3
1	G	224	LYS	4.3
2	H	83	ALA	4.3
2	H	180	LEU	4.2
2	F	169	ASN	4.2
1	C	111	SER	4.2
1	C	149	GLY	4.1
2	D	188	HIS	4.1
2	F	127	ALA	4.1
2	D	191	TYR	4.1
1	E	207	GLN	4.1
2	D	190	SER	4.1
1	G	106	PRO	4.1
2	H	125	LEU	4.0
2	H	79	ALA	4.0
2	H	114	SER	4.0
2	H	140	TYR	4.0
2	D	200	SER	4.0
1	G	59	TYR	4.0
2	H	185	TRP	3.9
1	C	57	TYR	3.9
2	D	209	THR	3.9
1	E	229	LYS	3.9
2	D	33	CYS	3.9
1	G	76	ARG	3.9
2	B	99	THR	3.8
1	C	101	LEU	3.8
1	G	110	VAL	3.8
2	H	187	SER	3.7
1	A	54	ASP	3.7
2	H	106	LEU	3.7
2	D	14	PRO	3.7
1	C	59	TYR	3.7
1	G	29	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	10	VAL	3.6
2	D	69	THR	3.6
2	H	117	LEU	3.6
1	C	55	GLY	3.6
1	G	200	PRO	3.5
2	H	192	SER	3.5
2	D	169	ASN	3.5
2	D	16	GLN	3.5
2	D	93	SER	3.5
2	D	52	LYS	3.5
2	D	206	VAL	3.5
2	H	188	HIS	3.5
2	D	157	ALA	3.5
1	C	56	GLY	3.5
2	B	180	LEU	3.5
1	G	6	GLU	3.5
1	G	79	LEU	3.4
2	H	186	LYS	3.4
1	G	222	VAL	3.4
1	G	130	SER	3.4
1	G	192	SER	3.4
2	H	13	SER	3.4
2	B	183	GLU	3.4
2	H	111	ALA	3.4
2	D	105	VAL	3.4
2	H	173	ALA	3.4
2	H	193	CYS	3.3
2	B	187	SER	3.3
2	H	146	VAL	3.3
2	H	132	LEU	3.3
1	G	229	LYS	3.3
1	G	73	ASP	3.3
2	D	181	THR	3.3
2	H	92	SER	3.3
1	G	92	ALA	3.3
2	H	128	ASN	3.3
1	C	30	SER	3.3
1	G	111	SER	3.2
2	D	199	GLY	3.2
1	C	151	ALA	3.2
2	H	127	ALA	3.2
2	H	16	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	205	THR	3.2
1	E	155	CYS	3.2
1	G	105	LEU	3.2
1	G	228	PRO	3.2
1	G	24	ALA	3.1
1	G	141	PRO	3.1
1	G	152	ALA	3.1
2	D	151	ASP	3.1
2	H	207	ALA	3.1
2	B	93	SER	3.1
2	D	75	SER	3.1
1	G	8	GLY	3.1
1	E	1	GLN	3.1
1	G	1	GLN	3.1
2	B	208	PRO	3.1
1	C	152	ALA	3.1
1	E	151	ALA	3.1
2	H	159	VAL	3.1
1	G	70	ILE	3.1
1	G	25	SER	3.1
2	H	201	THR	3.0
2	D	95	VAL	3.0
2	D	202	VAL	3.0
1	G	11	VAL	3.0
1	G	205	GLY	3.0
1	G	190	LEU	3.0
1	G	206	THR	3.0
2	H	50	ASP	3.0
1	C	53	PHE	3.0
2	D	132	LEU	2.9
2	H	155	VAL	2.9
1	C	66	GLY	2.9
1	G	80	HIS	2.9
1	C	82	HIS	2.9
2	D	145	THR	2.9
2	F	201	THR	2.9
2	D	170	ASN	2.9
1	C	207	GLN	2.9
2	H	164	PRO	2.9
2	D	48	TYR	2.9
2	D	137	SER	2.9
2	D	197	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	18	LEU	2.8
2	D	189	ARG	2.8
1	C	155	CYS	2.8
2	H	202	VAL	2.8
1	C	198	THR	2.8
1	G	150	THR	2.8
2	D	99	THR	2.8
2	B	186	LYS	2.8
2	D	207	ALA	2.8
1	C	199	VAL	2.8
1	G	157	VAL	2.8
2	H	17	THR	2.8
2	H	54	PRO	2.8
2	H	9	SER	2.8
1	E	107	PHE	2.8
1	G	140	ALA	2.8
2	D	203	GLU	2.8
2	D	201	THR	2.8
1	A	53	PHE	2.8
2	H	118	PHE	2.8
2	D	140	TYR	2.8
2	F	209	THR	2.8
2	H	115	VAL	2.8
2	D	66	SER	2.7
2	D	152	SER	2.7
2	H	55	SER	2.7
1	G	99	ASP	2.7
2	F	40	GLY	2.7
2	H	18	ALA	2.7
2	H	130	ALA	2.7
1	G	5	VAL	2.7
2	H	44	VAL	2.7
2	H	195	VAL	2.7
1	G	96	CYS	2.7
1	C	75	SER	2.7
2	B	122	SER	2.7
2	D	127	ALA	2.7
1	E	204	LEU	2.7
2	B	181	THR	2.7
2	D	131	THR	2.7
1	C	141	PRO	2.7
2	D	159	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	168	SER	2.7
1	C	112	GLY	2.7
2	H	76	GLY	2.7
1	C	61	ALA	2.6
1	G	69	THR	2.6
2	D	208	PRO	2.6
1	C	32	TYR	2.6
2	D	187	SER	2.6
2	H	143	ALA	2.6
1	G	28	THR	2.6
2	D	109	PRO	2.6
2	H	154	PRO	2.6
1	G	142	SER	2.6
2	H	134	CYS	2.6
1	A	16	THR	2.6
2	H	77	THR	2.6
1	A	202	SER	2.6
2	B	152	SER	2.6
1	C	226	VAL	2.6
1	G	58	GLN	2.6
2	D	184	GLN	2.6
1	A	22	CYS	2.6
2	H	104	THR	2.6
2	H	147	ALA	2.6
2	H	150	ALA	2.6
1	G	116	ASP	2.6
2	H	144	VAL	2.5
1	G	173	ALA	2.5
1	G	180	THR	2.5
1	G	7	SER	2.5
2	D	111	ALA	2.5
2	D	154	PRO	2.5
2	D	27	LEU	2.5
2	D	15	GLY	2.5
1	G	136	VAL	2.5
2	H	136	ILE	2.5
1	G	32	TYR	2.5
1	C	85	SER	2.5
1	C	192	SER	2.5
2	H	153	SER	2.5
2	H	163	THR	2.5
1	A	173	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	129	ALA	2.5
2	B	127	ALA	2.5
2	D	79	ALA	2.5
1	G	20	LEU	2.5
1	G	139	LEU	2.5
1	G	185	LEU	2.5
2	H	135	LEU	2.5
1	G	170	ASN	2.5
2	F	128	ASN	2.5
1	G	186	GLN	2.4
1	C	211	CYS	2.4
1	G	30	SER	2.4
2	D	122	SER	2.4
2	F	190	SER	2.4
2	H	179	SER	2.4
2	H	200	SER	2.4
2	D	180	LEU	2.4
2	H	78	GLN	2.4
2	H	105	VAL	2.4
1	G	17	SER	2.4
1	G	191	TYR	2.4
1	G	221	LYS	2.4
1	G	154	GLY	2.4
1	G	135	SER	2.4
1	G	169	TRP	2.4
1	G	78	THR	2.4
1	G	208	THR	2.4
2	D	129	LYS	2.4
2	F	189	ARG	2.4
2	H	189	ARG	2.4
2	H	113	PRO	2.4
2	F	125	LEU	2.4
2	D	59	GLU	2.4
1	C	113	GLY	2.4
2	D	24	GLY	2.4
2	H	56	GLY	2.4
2	H	169	ASN	2.4
1	G	127	SER	2.4
2	D	114	SER	2.4
2	D	34	TRP	2.4
2	D	147	ALA	2.3
2	D	117	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	100	GLY	2.3
2	D	149	LYS	2.3
1	G	51	ILE	2.3
2	D	182	PRO	2.3
2	H	182	PRO	2.3
1	C	96	CYS	2.3
2	H	31	TYR	2.3
2	H	112	ALA	2.3
1	G	214	ASN	2.3
1	A	79	LEU	2.3
2	D	50	ASP	2.3
2	H	139	PHE	2.3
1	A	203	SER	2.3
1	G	75	SER	2.3
2	D	92	SER	2.3
1	C	52	THR	2.3
1	E	3	GLN	2.3
2	H	145	THR	2.3
1	G	22	CYS	2.3
1	G	61	ALA	2.3
1	G	183	ALA	2.3
1	A	149	GLY	2.3
1	C	123	LEU	2.3
1	G	66	GLY	2.3
1	G	121	GLY	2.3
2	H	107	GLY	2.3
2	H	172	TYR	2.3
1	G	21	SER	2.3
1	G	2	VAL	2.3
1	G	122	THR	2.3
2	B	50	ASP	2.3
2	B	151	ASP	2.3
2	H	151	ASP	2.3
1	G	81	LEU	2.3
1	G	209	TYR	2.3
2	D	198	GLU	2.2
2	H	74	ILE	2.2
2	B	163	THR	2.2
2	D	58	PRO	2.2
2	F	186	LYS	2.2
2	H	191	TYR	2.2
1	G	188	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	162	THR	2.2
1	G	93	VAL	2.2
1	C	205	GLY	2.2
2	H	15	GLY	2.2
2	F	150	ALA	2.2
2	D	72	LEU	2.2
2	D	126	GLN	2.2
2	F	126	GLN	2.2
1	C	176	SER	2.2
1	G	85	SER	2.2
2	H	23	SER	2.2
1	A	109	TRP	2.2
2	B	209	THR	2.2
1	G	124	VAL	2.2
2	D	98	GLY	2.2
2	F	78	GLN	2.2
1	A	104	LEU	2.2
1	C	79	LEU	2.2
1	G	156	LEU	2.2
2	D	87	CYS	2.2
2	D	178	LEU	2.2
2	D	192	SER	2.2
2	H	75	SER	2.2
2	H	148	TRP	2.2
1	C	166	THR	2.2
1	G	125	THR	2.2
2	D	17	THR	2.2
2	H	14	PRO	2.1
2	H	119	PRO	2.1
1	E	196	VAL	2.1
2	F	12	VAL	2.1
2	D	194	GLN	2.1
1	E	173	ALA	2.1
1	G	101	LEU	2.1
2	D	134	CYS	2.1
2	D	23	SER	2.1
2	D	183	GLU	2.1
2	H	25	ASP	2.1
2	D	73	THR	2.1
2	D	148	TRP	2.1
2	B	155	VAL	2.1
1	G	104	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	153	SER	2.1
2	H	33	CYS	2.1
1	E	219	ASN	2.1
1	G	117	TYR	2.1
1	E	175	THR	2.1
1	G	138	PRO	2.1
1	E	109	TRP	2.1
1	G	53	PHE	2.1
2	D	155	VAL	2.1
1	A	30	SER	2.1
2	B	170	ASN	2.1
1	C	1	GLN	2.1
2	H	184	GLN	2.1
2	H	5	THR	2.1
1	G	112	GLY	2.1
2	D	204	LYS	2.1
2	H	129	LYS	2.1
1	A	107	PHE	2.1
1	G	199	VAL	2.1
1	A	142	SER	2.1
1	C	187	SER	2.1
2	F	23	SER	2.1
1	C	58	GLN	2.0
1	E	149	GLY	2.0
2	D	2	TYR	2.0
2	H	149	LYS	2.0
2	F	199	GLY	2.0
2	F	155	VAL	2.0
2	H	206	VAL	2.0
1	C	203	SER	2.0
1	G	203	SER	2.0
2	D	128	ASN	2.0
1	A	99	ASP	2.0
2	H	60	ARG	2.0
1	A	78	THR	2.0
1	C	69	THR	2.0
2	B	131	THR	2.0
2	D	104	THR	2.0
2	H	131	THR	2.0
1	G	26	GLY	2.0
2	D	40	GLY	2.0
1	C	60	TYR	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 oligosaccharides 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.