WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2023 – 05:05 PM EDT

PDB ID	:	4XCE
Title	:	Crystal structure of human 4E10 Fab crystalized in the presence of Phosphatidylcholine (06:0 PC); C2 space group
Authors	:	Irimia, A.; Stanfield, R.L.; Wilson, I.A.
Deposited on	:	2014-12-17
Resolution	:	2.93 Å(reported)

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

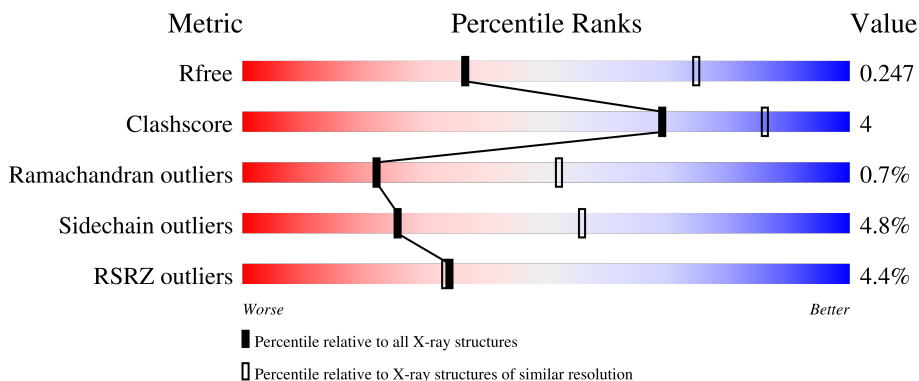|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.93 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.
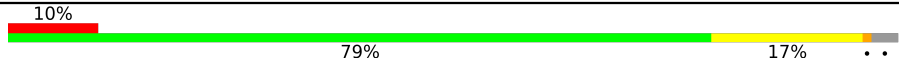
Metric	Percentile Ranks	Value
Rfree		0.247
Clashscore		4
Ramachandran outliers		0.7%
Sidechain outliers		4.8%
RSRZ outliers		4.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	B	215	90% 9%
1	D	215	88% 11%
1	L	215	90% 8%
2	A	230	83% 14%
2	C	230	83% 13%

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Mol	Chain	Length	Quality of chain
2	H	230	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9710 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 4E10 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	1	0
			1554	969	265	315	5			
1	B	214	Total	C	N	O	S	0	1	0
			1604	995	277	327	5			
1	D	214	Total	C	N	O	S	0	2	0
			1637	1016	283	333	5			

- Molecule 2 is a protein called 4E10 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	223	Total	C	N	O	S	0	5	0
			1605	1009	273	314	9			
2	A	225	Total	C	N	O	S	0	3	0
			1646	1042	278	318	8			
2	C	224	Total	C	N	O	S	0	3	0
			1616	1021	272	314	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	8	Total	O	0	0
			8	8		
3	H	3	Total	O	0	0
			3	3		
3	B	16	Total	O	0	0
			16	16		
3	A	8	Total	O	0	0
			8	8		
3	D	9	Total	O	0	0
			9	9		
3	C	4	Total	O	0	0
			4	4		

3 Residue-property plots ⓘ

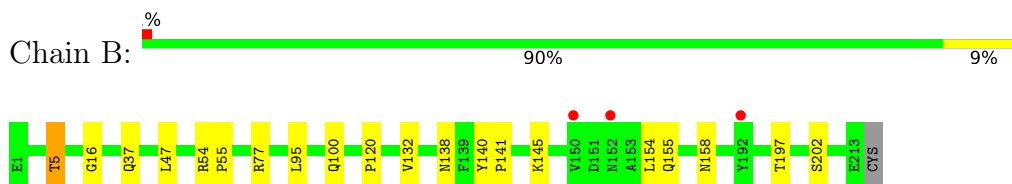These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4E10 Fab light chain

Chain L:

• Molecule 1: 4E10 Fab light chain

Chain B:

• Molecule 1: 4E10 Fab light chain

Chain D:

• Molecule 2: 4E10 Fab heavy chain

Chain H:

• Molecule 2: 4E10 Fab heavy chain

Chain A:

Chain A residue bar: Q1 V11 K23 A24 S25 F29 S30 T31 Y32 A33 L34 W47 I52 R66 A71 S76 T87 C92 A93 R94 W100B L100C G100D F100J T110 V111 S112 P119 S120 V121 F122 P123 P126 SER SER K129 S130 T133 S134 G135 G136 L140 Y147

F148 P149 V152 S195 L198 I207 V219 D220 K221 K222 V225 E226 P227 LYS SER CYS

• Molecule 2: 4E10 Fab heavy chain

Chain C:

Chain C residue bar: GLN V2 Q3 L4 E10 V11 P14 G15 S16 S17 A24 S25 S28 F29 S30 T31 L34 P52A T55 F63 I67 A71 L80 T87 C92 E95 G96 T97 G100A W100B L100C G100D K100E F100J T110 V111 S112 S113 P119 S127 SER

LYS SER THR SER G135 Y147 F148 P149 V152 L198 N209 D220 S229 C230

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	95.52Å　　164.31Å　　106.99Å 90.00°　　106.68°　　90.00°	Depositor
Resolution (Å)	46.99　－　2.93 46.99　－　2.93	Depositor EDS
% Data completeness (in resolution range)	93.4 (46.99-2.93) 93.4 (46.99-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.192　,　0.247 0.195　,　0.247	Depositor DCC
R_{free} test set	1592 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	63.2	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9710	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	B	0.26	0/1640	0.48	0/2233
1	D	0.25	0/1673	0.46	0/2271
1	L	0.25	0/1589	0.50	0/2167
2	A	0.25	0/1695	0.49	0/2318
2	C	0.26	0/1666	0.49	1/2286 (0.0%)
2	H	0.25	0/1658	0.53	0/2274
All	All	0.25	0/9921	0.49	1/13549 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	100(A)	GLY	N-CA-C	-5.37	99.69	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1604	0	1507	11	0
1	D	1637	0	1575	10	0
1	L	1554	0	1431	7	0
2	A	1646	0	1613	12	0
2	C	1616	0	1539	16	0
2	H	1605	0	1527	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	0	0	0
3	B	16	0	0	1	0
3	C	4	0	0	0	0
3	D	9	0	0	0	0
3	H	3	0	0	0	0
3	L	8	0	0	0	0
All	All	9710	0	9192	69	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 4.

All (69) 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:37:GLN:OE1	1:L:39:ARG:NH1	2.21	0.72
1:B:95:LEU:HD12	2:A:47:TRP:HZ3	1.57	0.69
1:L:5:THR:HG22	1:L:100:GLN:HE22	1.59	0.68
2:C:209:ASN:ND2	2:C:220:ASP:OD1	2.24	0.67
2:A:100(B):TRP:O	2:A:100(D):GLY:N	2.28	0.66
1:B:120:PRO:HD3	1:B:132:VAL:HG22	1.78	0.65
1:B:5:THR:HG22	1:B:100:GLN:HE22	1.63	0.64
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.79	0.64
2:H:87:THR:HG23	2:H:110:THR:HA	1.81	0.63
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.82	0.62
2:C:25:SER:OG	2:C:25:SER:O	2.14	0.60
1:B:37:GLN:HB2	1:B:47:LEU:HD11	1.83	0.59
2:H:29:PHE:O	2:H:52(A):PRO:HG2	2.02	0.59
1:B:95:LEU:HD12	2:A:47:TRP:CZ3	2.38	0.58
2:H:124:LEU:HD21	2:H:143:LEU:HB2	1.86	0.58
2:H:53:LEU:O	2:H:55:THR:HA	2.02	0.58
1:D:32:LYS:HD2	1:D:91:TYR:CE2	2.40	0.57
2:C:87:THR:HG23	2:C:110:THR:HA	1.86	0.57
1:D:37:GLN:HB2	1:D:47:LEU:HD11	1.88	0.56
2:H:212:HIS:CD2	2:H:214:PRO:HD2	2.41	0.55
2:C:67:ILE:HD11	2:C:80:LEU:HD11	1.90	0.54
2:A:93:ALA:HB1	2:A:100(J):PHE:HB3	1.90	0.54
1:D:185:ASP:OD1	1:D:188:LYS:NZ	2.33	0.53
2:C:11:VAL:HG21	2:C:149:PRO:HG3	1.90	0.52
2:C:34:LEU:HD11	2:C:92[B]:CYS:SG	2.50	0.51
2:A:135:GLY:H	2:A:195:SER:HB2	1.76	0.51
2:C:28:SER:HG	2:C:31:THR:HG1	1.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:PRO:HD3	1:D:132:VAL:HG22	1.91	0.50
1:B:155:GLN:NE2	3:B:313:HOH:O	2.30	0.50
2:A:34:LEU:HD11	2:A:92[B]:CYS:SG	2.52	0.50
1:B:145:LYS:HB3	1:B:197:THR:HB	1.95	0.49
2:H:93:ALA:HB1	2:H:100(J):PHE:HB3	1.95	0.48
2:H:11:VAL:HG21	2:H:149:PRO:HG3	1.94	0.48
2:A:121:VAL:O	2:A:221:LYS:NZ	2.34	0.48
2:H:30:SER:HA	2:H:52(A):PRO:HB2	1.96	0.47
2:C:119:PRO:HB3	2:C:147:TYR:HB3	1.95	0.47
1:B:16:GLY:O	1:B:77:ARG:HG3	2.15	0.47
2:H:40:ALA:HB3	2:H:43:ARG:HG3	1.97	0.46
2:C:30:SER:HA	2:C:52(A):PRO:HB2	1.98	0.45
1:L:113:PRO:HD3	1:L:198:HIS:ND1	2.32	0.45
2:A:123:PRO:HD3	2:A:221:LYS:HZ2	1.81	0.45
1:D:32:LYS:HG3	1:D:92:GLY:HA2	1.98	0.45
1:B:155:GLN:OE1	1:B:158:ASN:ND2	2.49	0.45
2:A:11:VAL:HG21	2:A:149:PRO:HG3	1.98	0.44
2:H:171:VAL:HA	2:H:191:VAL:HG23	2.00	0.44
2:H:112:SER:OG	2:H:113:SER:N	2.51	0.43
2:C:14:PRO:HD3	2:C:112:SER:O	2.17	0.43
1:L:145:LYS:HB2	1:L:197:THR:HB	2.01	0.43
2:A:119:PRO:HB3	2:A:147:TYR:HB3	2.01	0.43
1:D:38:GLN:O	1:D:84:ALA:HB1	2.19	0.42
1:D:16:GLY:O	1:D:77:ARG:HG3	2.19	0.42
1:D:35:TRP:CD2	1:D:73:LEU:HB2	2.54	0.42
2:C:63:PHE:O	2:C:67:ILE:HG22	2.20	0.42
2:C:95:GLU:HA	2:C:100(J):PHE:HA	2.01	0.42
2:C:16:SER:OG	2:C:17:SER:N	2.53	0.42
2:C:112:SER:OG	2:C:113:SER:N	2.52	0.42
1:D:118:PHE:HA	1:D:119:PRO:HD3	1.85	0.41
1:L:183:LYS:HB3	1:L:183:LYS:HE2	1.80	0.41
1:B:140:TYR:CG	1:B:141:PRO:HA	2.55	0.41
1:D:79:GLU:HG3	1:D:80:PRO:HD2	2.03	0.41
2:H:52(A):PRO:O	2:H:55:THR:HG22	2.21	0.41
2:A:87:THR:HG23	2:A:110:THR:HA	2.03	0.41
2:H:100(E):LYS:HA	2:H:100(F):PRO:HD3	1.85	0.41
1:L:108:ARG:NE	1:L:109:THR:O	2.48	0.40
2:H:144:VAL:HG11	2:H:152:VAL:HG11	2.02	0.40
1:B:54:ARG:HA	1:B:55:PRO:HD3	1.90	0.40
2:A:32:TYR:HD2	2:A:94:ARG:NH2	2.19	0.40
2:C:100(D):GLY:HA3	2:C:100(E):LYS:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:LEU:HD13	2:C:92[B]:CYS:SG	2.62	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	B	213/215 (99%)	204 (96%)	8 (4%)	1 (0%)	29	60
1	D	214/215 (100%)	204 (95%)	10 (5%)	0	100	100
1	L	209/215 (97%)	196 (94%)	12 (6%)	1 (0%)	29	60
2	A	224/230 (97%)	211 (94%)	10 (4%)	3 (1%)	12	35
2	C	223/230 (97%)	215 (96%)	8 (4%)	0	100	100
2	H	222/230 (96%)	212 (96%)	6 (3%)	4 (2%)	8	27
All	All	1305/1335 (98%)	1242 (95%)	54 (4%)	9 (1%)	22	52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	72	ASP
2	A	100(C)	LEU
2	H	54	LEU
2	H	100(A)	GLY
2	A	29	PHE
2	A	134	SER
2	H	71	ALA
1	L	138	ASN
1	B	138	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	174/185 (94%)	171 (98%)	3 (2%)	60	83
1	D	183/185 (99%)	178 (97%)	5 (3%)	44	74
1	L	162/185 (88%)	154 (95%)	8 (5%)	25	55
2	A	180/189 (95%)	168 (93%)	12 (7%)	16	41
2	C	173/189 (92%)	164 (95%)	9 (5%)	23	53
2	H	173/189 (92%)	161 (93%)	12 (7%)	15	40
All	All	1045/1122 (93%)	996 (95%)	49 (5%)	25	57

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	14	SER
1	L	22	SER
1	L	39	ARG
1	L	129	THR
1	L	133	VAL
1	L	176	SER
1	L	179	LEU
2	H	23	LYS
2	H	31	THR
2	H	34	LEU
2	H	68	THR
2	H	82(A)	ASN
2	H	83	ARG
2	H	97	THR
2	H	100(C)	LEU
2	H	143	LEU
2	H	191	VAL
2	H	200	THR
2	H	230	CYS
1	B	5	THR
1	B	154	LEU

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Mol	Chain	Res	Type
1	B	202	SER
2	A	1	GLN
2	A	31	THR
2	A	34	LEU
2	A	52	ILE
2	A	66	ARG
2	A	76	SER
2	A	112	SER
2	A	140	LEU
2	A	152	VAL
2	A	198	LEU
2	A	207	ILE
2	A	219	VAL
1	D	20	THR
1	D	33	LEU
1	D	60	ASP
1	D	72	THR
1	D	154	LEU
2	C	10	GLU
2	C	25	SER
2	C	31	THR
2	C	34	LEU
2	C	55	THR
2	C	97	THR
2	C	100(B)	TRP
2	C	110	THR
2	C	152	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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, 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	B	214/215 (99%)	0.08	3 (1%)	75	77	34, 56, 99, 123	0
1	D	214/215 (99%)	0.01	1 (0%)	91	91	34, 61, 85, 134	0
1	L	212/215 (98%)	0.34	15 (7%)	16	14	38, 68, 137, 150	0
2	A	225/230 (97%)	0.16	11 (4%)	29	29	39, 66, 108, 144	0
2	C	224/230 (97%)	0.23	5 (2%)	62	63	42, 75, 114, 143	0
2	H	223/230 (96%)	0.48	23 (10%)	6	6	44, 87, 138, 153	0
All	All	1312/1335 (98%)	0.22	58 (4%)	34	33	34, 69, 127, 153	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	135	GLY	8.0
2	H	230	CYS	6.8
1	L	209	PHE	6.5
2	H	127	SER	5.6
1	D	213	GLU	5.5
2	H	100(B)	TRP	5.4
1	L	191	VAL	4.9
1	L	212	GLY	4.8
1	L	192	TYR	4.6
1	L	194[A]	CYS	4.5
2	A	134	SER	4.5
2	H	140	LEU	4.4
2	C	229	SER	4.2
2	A	130	SER	4.2
2	H	126	PRO	4.1
2	C	198	LEU	3.9
2	H	211	ASN	3.8
1	L	210	ASN	3.7
2	A	198	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	205	THR	3.4
2	H	141	GLY	3.4
2	H	123	PRO	3.4
1	L	186	TYR	3.4
2	H	100(A)	GLY	3.3
2	C	71	ALA	3.3
2	H	207	ILE	3.2
2	H	219	VAL	3.0
1	L	211	ARG	3.0
1	B	192	TYR	3.0
2	H	220	ASP	2.9
2	A	129	LYS	2.9
2	A	23	LYS	2.8
2	H	122	PHE	2.8
2	A	136	GLY	2.8
1	L	122	ASP	2.7
1	L	133	VAL	2.7
1	L	116	PHE	2.6
2	H	200	THR	2.6
1	B	150	VAL	2.6
2	H	227	PRO	2.6
2	H	142[A]	CYS	2.5
2	H	229	SER	2.4
2	H	154	VAL	2.4
2	H	153	THR	2.4
2	H	25	SER	2.3
2	H	139	ALA	2.3
2	A	71	ALA	2.3
1	L	121	SER	2.2
2	A	140	LEU	2.2
1	L	123	GLU	2.2
2	C	34	LEU	2.2
2	A	25	SER	2.2
1	L	152	ASN	2.1
1	B	152	ASN	2.1
2	C	24	ALA	2.1
2	H	193	VAL	2.1
1	L	200	GLY	2.0
2	A	225	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides 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.