Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2026 – 06:27 PM EDT

PDB ID	:	38DC / pdb_000038dc
Title	:	X-ray Structure of the FAB Fragment of a GluA2-specific Murine Monoclonal Antibody 15F1
Authors	:	Nix, J.; Dhandapani, G.; Spangler, C.J.; Pruneda, J.N.; Gouaux, E.
Deposited on	:	2026-08-20
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
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:

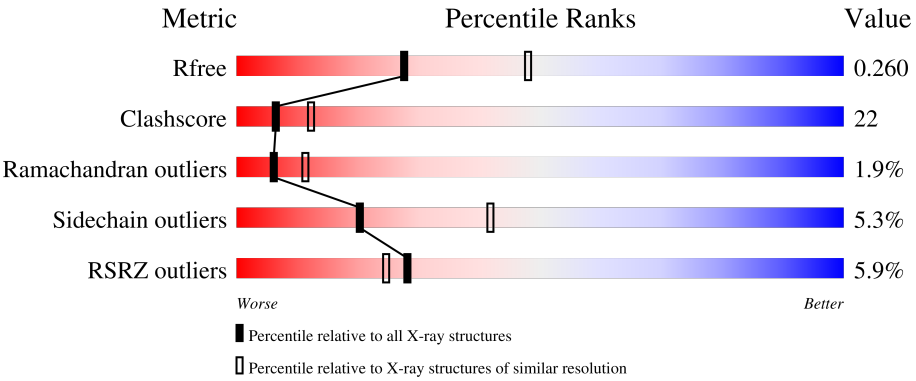
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	A	233	7% 58% 36%
1	C	233	9% 56% 35% 6%
2	B	216	3% 75% 22%
2	D	216	5% 59% 38%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13417 atoms, of which 6505 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 15F1 Fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	227	Total	C	H	N	O	S	0	0	0
			3316	1059	1637	280	331	9			
1	C	227	Total	C	H	N	O	S	0	0	0
			3354	1075	1653	281	336	9			

- Molecule 2 is a protein called 15F1 Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	216	Total	C	H	N	O	S	0	0	0
			3287	1041	1607	284	348	7			
2	D	216	Total	C	H	N	O	S	0	0	0
			3289	1041	1608	284	349	7			

- Molecule 3 is water.

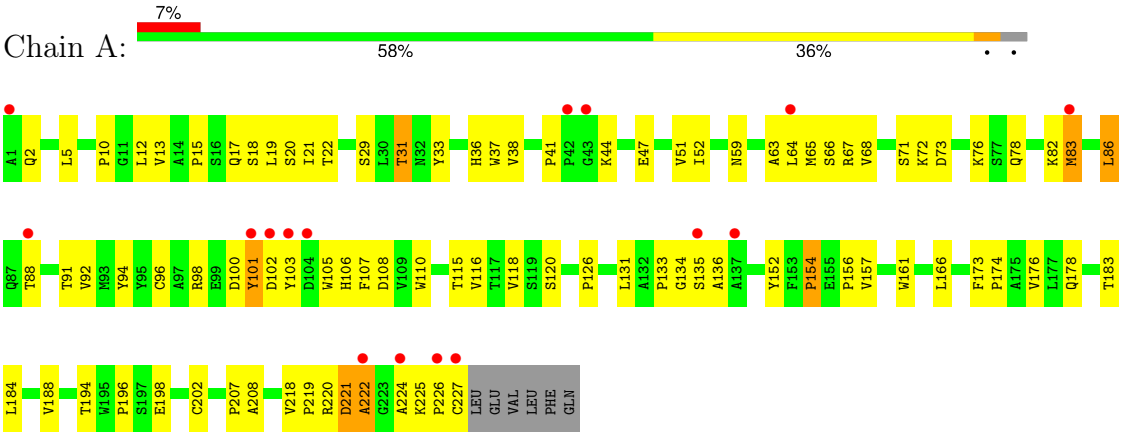
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	60	Total	O	0	0
			60	60		
3	C	46	Total	O	0	0
			46	46		
3	D	26	Total	O	0	0
			26	26		

3 Residue-property plots (i)

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

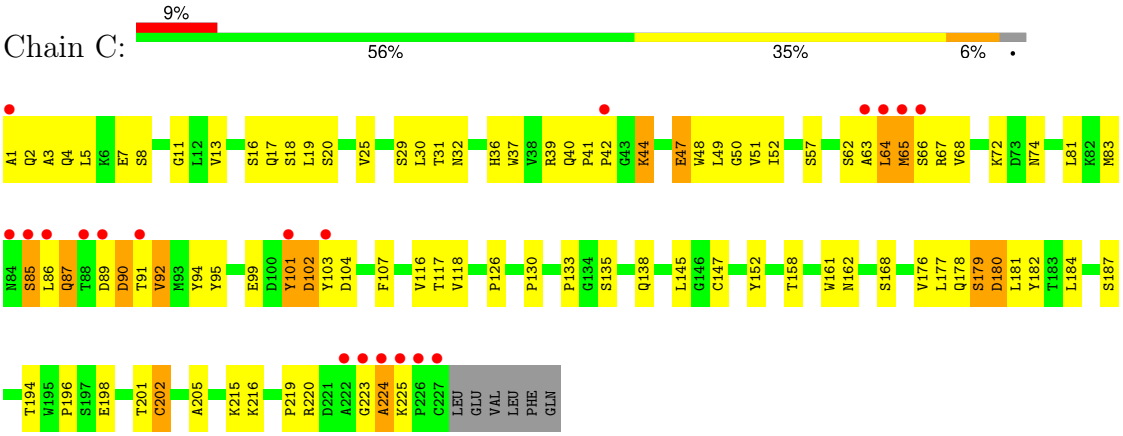
• Molecule 1: 15F1 Fab heavy chain

Chain A:



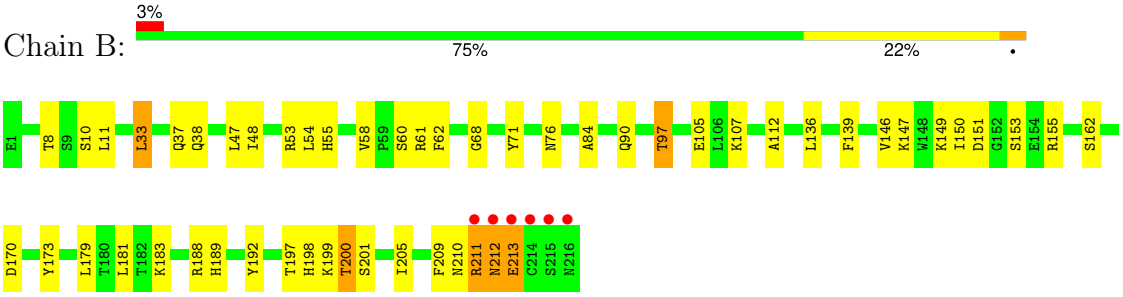
• Molecule 1: 15F1 Fab heavy chain

Chain C:



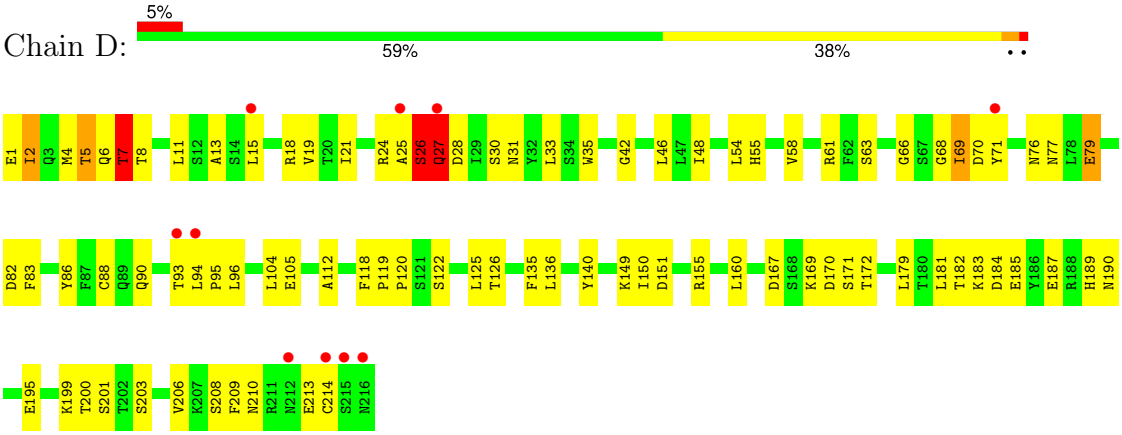
• Molecule 2: 15F1 Fab light chain

Chain B:



• Molecule 2: 15F1 Fab light chain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.46Å 64.28Å 204.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.09 – 2.50 46.09 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.09-2.50) 99.8 (46.09-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.82 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.209 , 0.257 0.212 , 0.260	Depositor DCC
R_{free} test set	2539 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13417	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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 24.22 % 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 4.0018e-03. 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, 0.333 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	0.79	2/1724 (0.1%)	1.03	1/2363 (0.0%)
1	C	0.72	0/1748	0.99	4/2396 (0.2%)
2	B	0.84	0/1714	1.04	1/2326 (0.0%)
2	D	0.72	2/1715 (0.1%)	0.92	1/2326 (0.0%)
All	All	0.77	4/6901 (0.1%)	1.00	7/9411 (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
2	D	0	3
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	MET	SD-CE	6.96	1.97	1.79
2	D	118	PHE	CA-C	-6.59	1.47	1.52
1	A	131	LEU	C-N	-5.38	1.04	1.34
2	D	27	GLN	CB-CG	5.10	1.67	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	64	LEU	N-CA-C	11.56	124.05	110.41
1	C	101	TYR	CA-C-N	-7.06	108.05	121.54
1	C	101	TYR	C-N-CA	-7.06	108.05	121.54
2	B	210	ASN	N-CA-C	-5.56	103.06	111.34
1	C	202	CYS	CA-CB-SG	5.55	127.16	114.40
1	A	83	MET	CG-SD-CE	-5.32	89.19	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	27	GLN	CB-CG-CD	5.28	121.57	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	85	SER	Peptide
2	D	18	ARG	Sidechain
2	D	2	ILE	Peptide
2	D	26	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1679	1637	1629	91	0
1	C	1701	1653	1653	84	0
2	B	1680	1607	1607	49	1
2	D	1681	1608	1607	83	1
3	A	39	0	0	4	0
3	B	60	0	0	9	0
3	C	46	0	0	9	0
3	D	26	0	0	1	0
All	All	6912	6505	6496	290	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 22.

All (290) 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:D:2:ILE:HG22	2:D:27:GLN:NE2	1.69	1.06
2:D:182:THR:HG22	2:D:184:ASP:H	1.20	1.06
2:D:2:ILE:HG22	2:D:27:GLN:CD	1.86	0.98
1:C:201:THR:HG22	1:C:216:LYS:HG3	1.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:PRO:O	3:C:301:HOH:O	1.88	0.90
1:A:100:ASP:O	3:A:301:HOH:O	1.90	0.89
1:C:63:ALA:O	1:C:67:ARG:NH2	2.06	0.88
2:D:55:HIS:O	2:D:58:VAL:HG12	1.76	0.86
1:A:68:VAL:HG22	1:A:83:MET:HG2	1.56	0.85
1:C:180:ASP:OD1	3:C:302:HOH:O	1.94	0.85
2:D:76:ASN:ND2	2:D:77:ASN:OD1	2.09	0.84
2:B:198:HIS:ND1	2:B:200:THR:HB	1.94	0.83
2:B:155:ARG:O	3:B:301:HOH:O	1.97	0.83
2:D:199:LYS:NZ	3:D:301:HOH:O	2.10	0.83
1:A:83:MET:HE1	1:A:94:TYR:CZ	2.15	0.81
2:B:183:LYS:NZ	3:B:302:HOH:O	1.99	0.80
1:A:102:ASP:HB3	3:A:302:HOH:O	1.81	0.80
2:B:105:GLU:OE1	2:B:173:TYR:OH	1.99	0.80
1:C:13:VAL:HG23	1:C:118:VAL:HG22	1.64	0.78
2:D:5:THR:HG23	2:D:24:ARG:HB2	1.64	0.77
1:A:64:LEU:HD12	1:A:67:ARG:HE	1.50	0.74
2:B:107:LYS:O	3:B:303:HOH:O	2.03	0.74
1:C:220:ARG:NH2	2:D:120:PRO:O	2.20	0.74
1:C:40:GLN:NE2	3:C:303:HOH:O	2.14	0.74
2:D:150:ILE:HD11	2:D:179:LEU:HD21	1.69	0.74
1:C:101:TYR:O	1:C:103:TYR:N	2.21	0.73
1:C:215:LYS:NZ	3:C:305:HOH:O	2.18	0.73
2:D:54:LEU:HG	2:D:58:VAL:HG13	1.72	0.72
1:C:52:ILE:HD13	1:C:72:LYS:HB3	1.69	0.72
2:D:182:THR:HG22	2:D:184:ASP:N	2.01	0.72
1:A:13:VAL:HG23	1:A:118:VAL:HG22	1.73	0.68
1:A:126:PRO:HB3	1:A:152:TYR:HB3	1.74	0.68
1:C:196:PRO:HG3	1:C:219:PRO:HG3	1.73	0.68
1:C:62:SER:H	2:D:95:PRO:HG3	1.58	0.68
1:A:100:ASP:HB2	1:A:108:ASP:CG	2.20	0.67
2:B:189:HIS:O	2:B:211:ARG:NH2	2.29	0.66
2:D:31:ASN:HA	2:D:71:TYR:HE2	1.61	0.66
1:A:102:ASP:O	1:A:103:TYR:CB	2.44	0.66
1:A:17:GLN:C	1:A:86:LEU:HD12	2.21	0.65
1:C:225:LYS:NZ	3:C:308:HOH:O	2.29	0.65
1:A:220:ARG:O	1:A:221:ASP:C	2.40	0.64
1:C:19:LEU:HD23	1:C:83:MET:HG3	1.79	0.64
1:A:135:SER:HB2	2:B:213:GLU:HG3	1.79	0.64
1:C:13:VAL:CG2	1:C:118:VAL:HG22	2.27	0.64
1:C:177:LEU:HD12	1:C:181:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:THR:CG2	1:C:216:LYS:HG3	2.27	0.63
1:C:62:SER:C	1:C:65:MET:HE1	2.24	0.63
1:C:225:LYS:HE2	3:C:308:HOH:O	1.98	0.62
2:D:122:SER:HA	2:D:125:LEU:HD12	1.82	0.62
1:A:135:SER:CB	2:B:213:GLU:HG3	2.30	0.62
1:A:83:MET:HE1	1:A:94:TYR:OH	2.00	0.61
2:B:205:ILE:H	2:B:205:ILE:HD12	1.65	0.61
1:C:177:LEU:HD13	1:C:182:TYR:CE1	2.36	0.61
2:D:170:ASP:OD1	2:D:170:ASP:C	2.43	0.61
2:D:135:PHE:C	2:D:136:LEU:HD12	2.26	0.60
1:C:52:ILE:HG23	1:C:52:ILE:O	2.01	0.60
1:A:51:VAL:HG22	1:A:52:ILE:N	2.17	0.59
2:D:61:ARG:NH1	2:D:79:GLU:HG3	2.16	0.59
1:C:17:GLN:HG2	1:C:18:SER:H	1.67	0.59
2:D:155:ARG:NH2	2:D:181:LEU:HD22	2.17	0.59
1:A:106:HIS:CE1	3:A:302:HOH:O	2.55	0.58
1:A:88:THR:O	1:A:118:VAL:HG11	2.03	0.58
1:C:87:GLN:O	1:C:118:VAL:HB	2.04	0.58
2:B:112:ALA:HA	2:B:200:THR:HG21	1.85	0.58
2:B:8:THR:HG21	2:B:11:LEU:HD13	1.85	0.58
1:A:17:GLN:O	1:A:86:LEU:HD12	2.03	0.57
1:C:177:LEU:HD13	1:C:182:TYR:CD1	2.40	0.56
1:C:225:LYS:CE	3:C:308:HOH:O	2.53	0.56
1:A:220:ARG:HG2	1:A:220:ARG:HH11	1.70	0.56
2:D:46:LEU:HD23	2:D:55:HIS:CG	2.41	0.56
2:D:61:ARG:CZ	2:D:79:GLU:HG3	2.35	0.56
1:C:86:LEU:HA	3:C:306:HOH:O	2.05	0.56
1:A:100:ASP:OD1	1:A:101:TYR:N	2.38	0.56
2:D:24:ARG:HH22	2:D:69:ILE:HD12	1.70	0.56
2:B:136:LEU:N	2:B:136:LEU:HD12	2.21	0.56
2:D:122:SER:O	2:D:126:THR:HG23	2.06	0.56
2:D:2:ILE:C	2:D:27:GLN:OE1	2.48	0.55
1:A:83:MET:HE1	1:A:94:TYR:CE1	2.41	0.55
2:B:105:GLU:OE1	2:B:173:TYR:CZ	2.59	0.55
2:D:94:LEU:HD12	2:D:94:LEU:H	1.71	0.55
1:A:63:ALA:O	1:A:64:LEU:HD13	2.06	0.55
2:D:105:GLU:OE2	2:D:140:TYR:OH	2.17	0.55
1:C:42:PRO:O	1:C:44:LYS:HD2	2.07	0.55
2:D:2:ILE:HD11	2:D:95:PRO:HD2	1.89	0.54
2:D:150:ILE:HD12	2:D:155:ARG:HD3	1.89	0.54
2:D:68:GLY:O	2:D:69:ILE:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG11	1:A:110:TRP:HZ3	1.72	0.54
1:C:19:LEU:HD23	1:C:83:MET:HB2	1.90	0.54
2:D:6:GLN:O	2:D:7:THR:C	2.49	0.54
1:A:220:ARG:O	1:A:222:ALA:N	2.41	0.54
1:C:19:LEU:HD23	1:C:83:MET:CG	2.38	0.54
2:D:2:ILE:HG21	2:D:93:THR:CG2	2.38	0.54
1:A:73:ASP:OD2	1:A:76:LYS:NZ	2.31	0.53
1:C:11:GLY:O	1:C:117:THR:N	2.34	0.53
1:A:21:ILE:HG22	1:A:37:TRP:CH2	2.43	0.53
1:A:71:SER:OG	1:A:82:LYS:NZ	2.41	0.53
1:A:29:SER:OG	1:A:31:THR:HB	2.09	0.53
1:A:133:PRO:O	1:A:220:ARG:HD2	2.09	0.53
1:C:95:TYR:OH	2:D:42:GLY:O	2.21	0.53
1:A:76:LYS:O	1:A:78:GLN:HG3	2.08	0.53
1:C:39:ARG:HG2	1:C:49:LEU:HD21	1.90	0.53
1:C:179:SER:OG	3:C:304:HOH:O	2.17	0.53
1:A:194:THR:O	1:A:198:GLU:HB2	2.08	0.53
2:D:13:ALA:HB2	2:D:19:VAL:HG21	1.91	0.53
1:A:220:ARG:HG2	1:A:220:ARG:NH1	2.24	0.53
1:C:92:VAL:HG22	1:C:94:TYR:CE1	2.44	0.53
2:D:6:GLN:NE2	2:D:86:TYR:O	2.36	0.53
1:C:89:ASP:C	1:C:91:THR:H	2.17	0.52
2:D:4:MET:SD	2:D:90:GLN:HB3	2.48	0.52
1:C:178:GLN:HB3	2:D:160:LEU:HD11	1.91	0.52
1:C:194:THR:O	1:C:198:GLU:HB2	2.10	0.52
1:C:36:HIS:NE2	1:C:99:GLU:OE1	2.40	0.52
1:A:154:PRO:HD2	1:A:208:ALA:CB	2.40	0.52
2:D:66:GLY:HA3	2:D:71:TYR:HA	1.91	0.52
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.92	0.52
2:D:24:ARG:NH1	2:D:24:ARG:HG2	2.24	0.52
1:A:64:LEU:HA	1:A:67:ARG:CZ	2.40	0.52
1:C:2:GLN:OE1	1:C:2:GLN:N	2.33	0.52
1:A:100:ASP:HB2	1:A:108:ASP:OD2	2.10	0.51
1:A:135:SER:OG	1:A:220:ARG:HB2	2.11	0.51
1:C:223:GLY:O	1:C:224:ALA:O	2.28	0.51
2:D:83:PHE:CD2	2:D:104:LEU:HD23	2.46	0.51
1:C:4:GLN:C	1:C:5:LEU:HD12	2.36	0.50
2:B:33:LEU:HD22	2:B:71:TYR:HB3	1.93	0.50
1:C:39:ARG:NH2	1:C:47:GLU:OE1	2.40	0.50
2:D:26:SER:HB3	2:D:27:GLN:OE1	2.11	0.50
2:D:24:ARG:HG2	2:D:24:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:TRP:CE2	1:C:81:LEU:HB2	2.47	0.50
2:D:54:LEU:HG	2:D:58:VAL:CG1	2.42	0.50
2:D:68:GLY:C	2:D:69:ILE:HG23	2.37	0.50
1:A:19:LEU:CD2	1:A:116:VAL:HG11	2.43	0.49
1:C:201:THR:HG22	1:C:216:LYS:CG	2.31	0.49
1:C:48:TRP:CZ2	1:C:50:GLY:HA2	2.47	0.49
1:A:135:SER:N	2:B:213:GLU:HG3	2.28	0.49
1:C:87:GLN:HG3	1:C:90:ASP:CG	2.37	0.49
1:A:36:HIS:CD2	1:A:107:PHE:HE1	2.30	0.49
1:A:100:ASP:O	1:A:102:ASP:N	2.46	0.49
1:A:207:PRO:O	1:A:208:ALA:C	2.56	0.49
2:B:90:GLN:HE21	2:B:97:THR:H	1.60	0.49
1:C:72:LYS:HD2	1:C:74:ASN:OD1	2.12	0.49
1:C:90:ASP:C	1:C:92:VAL:HG13	2.37	0.49
1:A:100:ASP:OD1	1:A:100:ASP:C	2.57	0.48
2:D:183:LYS:NZ	2:D:187:GLU:OE2	2.46	0.48
1:C:48:TRP:CE2	2:D:96:LEU:HD13	2.48	0.48
2:D:27:GLN:O	2:D:69:ILE:HG22	2.13	0.48
1:A:38:VAL:HG11	1:A:110:TRP:CZ3	2.48	0.48
1:A:38:VAL:HG23	1:A:47:GLU:C	2.39	0.48
2:D:48:ILE:HD13	2:D:54:LEU:HD12	1.94	0.48
2:B:33:LEU:HD22	2:B:71:TYR:CB	2.44	0.48
1:C:130:PRO:HD3	1:C:215:LYS:HE2	1.95	0.48
2:B:53:ARG:NE	3:B:304:HOH:O	2.17	0.48
1:A:196:PRO:CB	1:A:219:PRO:HG3	2.44	0.47
2:B:54:LEU:HD11	2:B:62:PHE:O	2.14	0.47
1:C:19:LEU:HD11	1:C:116:VAL:HG21	1.96	0.47
1:C:41:PRO:HB2	1:C:44:LYS:HD3	1.96	0.47
1:C:48:TRP:HZ2	1:C:51:VAL:HG12	1.78	0.47
2:D:151:ASP:OD2	2:D:189:HIS:ND1	2.40	0.47
2:D:149:LYS:HE3	2:D:195:GLU:OE1	2.15	0.47
2:D:15:LEU:HD23	2:D:83:PHE:HE1	1.80	0.47
2:D:71:TYR:CD1	2:D:71:TYR:N	2.81	0.47
1:C:101:TYR:C	1:C:103:TYR:H	2.22	0.47
2:D:31:ASN:HA	2:D:71:TYR:CE2	2.46	0.47
1:A:64:LEU:O	1:A:67:ARG:HG2	2.15	0.46
1:A:44:LYS:HD2	1:C:1:ALA:CB	2.45	0.46
1:C:30:LEU:HD12	1:C:74:ASN:HA	1.96	0.46
1:C:31:THR:O	1:C:31:THR:HG22	2.15	0.46
2:D:96:LEU:HD12	2:D:96:LEU:H	1.81	0.46
1:A:38:VAL:HG23	1:A:47:GLU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:HD2	1:C:1:ALA:HB2	1.97	0.46
1:C:158:THR:OG1	1:C:205:ALA:HB3	2.15	0.46
1:A:135:SER:CA	2:B:213:GLU:HG3	2.46	0.46
1:C:133:PRO:HD3	1:C:145:LEU:HD23	1.97	0.46
2:D:24:ARG:NH1	2:D:70:ASP:OD1	2.48	0.46
2:D:167:ASP:O	2:D:171:SER:HA	2.15	0.46
1:A:176:VAL:HG12	1:A:183:THR:O	2.15	0.46
2:D:69:ILE:HG13	2:D:70:ASP:OD1	2.16	0.46
2:B:48:ILE:CD1	2:B:54:LEU:HD12	2.46	0.46
2:B:105:GLU:OE1	2:B:173:TYR:CE1	2.68	0.46
2:D:119:PRO:HB3	2:D:209:PHE:CE2	2.51	0.46
2:D:2:ILE:CG2	2:D:27:GLN:CD	2.75	0.46
1:A:64:LEU:HD13	1:A:67:ARG:HH21	1.80	0.45
1:A:105:TRP:N	3:A:302:HOH:O	2.19	0.45
2:B:53:ARG:HG2	3:B:304:HOH:O	2.14	0.45
1:A:98:ARG:O	1:A:107:PHE:HA	2.16	0.45
2:B:170:ASP:C	2:B:170:ASP:OD1	2.59	0.45
2:D:1:GLU:HG2	2:D:2:ILE:H	1.81	0.45
2:B:61:ARG:HB2	2:B:76:ASN:O	2.16	0.45
2:D:35:TRP:N	2:D:48:ILE:O	2.39	0.45
1:A:19:LEU:HD22	1:A:116:VAL:HG11	1.99	0.45
1:C:89:ASP:O	1:C:91:THR:N	2.50	0.45
2:D:31:ASN:H	2:D:71:TYR:HH	1.62	0.45
1:C:102:ASP:OD1	1:C:104:ASP:HB2	2.16	0.45
1:C:68:VAL:HG22	1:C:83:MET:SD	2.57	0.45
1:C:64:LEU:C	1:C:64:LEU:HD12	2.41	0.45
2:D:24:ARG:HA	2:D:69:ILE:O	2.17	0.45
1:A:21:ILE:HG22	1:A:37:TRP:HH2	1.82	0.44
2:D:206:VAL:O	2:D:206:VAL:HG13	2.17	0.44
1:A:133:PRO:O	1:A:134:GLY:C	2.60	0.44
1:A:173:PHE:O	1:A:174:PRO:C	2.60	0.44
1:C:3:ALA:O	1:C:4:GLN:HG3	2.17	0.44
1:A:15:PRO:CD	1:A:120:SER:HB3	2.47	0.44
2:B:8:THR:HG21	2:B:11:LEU:CD1	2.48	0.44
2:B:53:ARG:CG	3:B:304:HOH:O	2.65	0.44
2:B:55:HIS:O	2:B:58:VAL:HG23	2.17	0.44
1:A:161:TRP:CH2	1:A:202:CYS:HB3	2.52	0.44
1:A:224:ALA:O	1:A:225:LYS:C	2.59	0.44
1:A:5:LEU:HB3	1:A:96:CYS:SG	2.58	0.44
2:D:105:GLU:O	2:D:105:GLU:HG3	2.14	0.44
1:A:65:MET:O	1:A:66:SER:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:ALA:N	2:D:200:THR:HG21	2.33	0.44
2:D:182:THR:HB	2:D:185:GLU:HG3	1.99	0.44
1:A:51:VAL:CG2	1:A:52:ILE:N	2.81	0.43
2:B:139:PHE:CE1	2:B:173:TYR:HB2	2.53	0.43
2:D:83:PHE:CE2	2:D:104:LEU:HD23	2.53	0.43
1:A:64:LEU:HA	1:A:67:ARG:NH2	2.33	0.43
1:A:91:THR:O	1:A:92:VAL:HG23	2.18	0.43
1:A:174:PRO:HD2	2:B:162:SER:OG	2.18	0.43
1:C:86:LEU:HB3	1:C:118:VAL:HG21	2.00	0.43
1:A:10:PRO:C	1:A:12:LEU:H	2.26	0.43
1:A:15:PRO:HA	1:A:86:LEU:O	2.18	0.43
1:A:41:PRO:HB2	1:A:44:LYS:HB2	2.01	0.43
2:B:150:ILE:HD12	2:B:192:TYR:CE2	2.52	0.43
1:A:36:HIS:CG	1:A:107:PHE:CE1	3.07	0.43
1:A:226:PRO:O	1:A:227:CYS:C	2.60	0.43
2:D:190:ASN:O	2:D:210:ASN:HA	2.18	0.43
1:A:184:LEU:HD12	1:A:184:LEU:C	2.43	0.43
2:B:197:THR:HA	3:B:330:HOH:O	2.18	0.43
1:C:29:SER:HB3	1:C:32:ASN:OD1	2.19	0.43
1:A:157:VAL:HG23	1:A:184:LEU:HD21	1.99	0.43
1:C:87:GLN:HG3	1:C:90:ASP:OD1	2.19	0.43
1:A:33:TYR:CG	1:A:98:ARG:HD2	2.53	0.43
1:C:13:VAL:O	1:C:118:VAL:HA	2.19	0.43
2:D:68:GLY:O	2:D:69:ILE:CG2	2.66	0.43
1:A:52:ILE:HG12	1:A:72:LYS:HG2	2.01	0.43
1:A:19:LEU:HD12	1:A:20:SER:N	2.34	0.43
1:C:177:LEU:HD12	1:C:181:LEU:C	2.43	0.43
1:C:19:LEU:HD12	1:C:20:SER:H	1.84	0.42
1:C:126:PRO:HB3	1:C:152:TYR:HB3	2.00	0.42
1:A:157:VAL:CG2	1:A:184:LEU:HD21	2.50	0.42
2:D:61:ARG:NH1	2:D:82:ASP:OD1	2.53	0.42
2:B:105:GLU:OE2	3:B:305:HOH:O	2.21	0.42
2:D:13:ALA:HB2	2:D:19:VAL:CG2	2.49	0.42
2:D:28:ASP:OD1	2:D:30:SER:N	2.52	0.42
1:A:134:GLY:C	2:B:213:GLU:OE2	2.63	0.42
1:A:178:GLN:OE1	1:A:178:GLN:HA	2.18	0.42
2:B:8:THR:HG22	2:B:10:SER:O	2.19	0.42
2:B:192:TYR:HB2	2:B:209:PHE:CE2	2.55	0.42
1:C:63:ALA:N	1:C:65:MET:HE1	2.34	0.42
1:C:161:TRP:O	1:C:162:ASN:C	2.62	0.42
2:D:25:ALA:HB3	2:D:69:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:ARG:HB3	2:B:212:ASN:OD1	2.20	0.42
2:D:167:ASP:OD1	2:D:169:LYS:HB2	2.19	0.42
1:C:107:PHE:N	1:C:107:PHE:CD2	2.85	0.42
1:C:19:LEU:HD23	1:C:83:MET:CB	2.49	0.42
1:C:29:SER:OG	1:C:31:THR:HB	2.19	0.42
1:C:52:ILE:O	1:C:52:ILE:CG2	2.68	0.42
1:C:2:GLN:H	1:C:2:GLN:CD	2.22	0.41
2:D:2:ILE:HG22	2:D:27:GLN:OE1	2.16	0.41
1:A:135:SER:HB2	2:B:213:GLU:CG	2.48	0.41
1:C:135:SER:HB2	2:D:214:CYS:HA	2.01	0.41
1:C:184:LEU:HD12	1:C:184:LEU:C	2.45	0.41
2:D:136:LEU:HD12	2:D:136:LEU:N	2.35	0.41
2:B:11:LEU:HD12	2:B:11:LEU:HA	1.92	0.41
1:A:91:THR:O	1:A:92:VAL:CG2	2.69	0.41
2:B:150:ILE:O	2:B:151:ASP:C	2.63	0.41
1:C:187:SER:HB3	2:D:135:PHE:CE2	2.55	0.41
1:A:161:TRP:HB3	1:A:166:LEU:HD12	2.01	0.41
2:B:47:LEU:HA	2:B:58:VAL:HG21	2.03	0.41
1:C:7:GLU:OE1	1:C:7:GLU:N	2.52	0.41
1:C:87:GLN:O	1:C:90:ASP:HB2	2.20	0.41
2:D:7:THR:OG1	2:D:8:THR:N	2.53	0.41
1:A:225:LYS:HE3	1:A:225:LYS:HB3	1.88	0.41
2:D:2:ILE:HG22	2:D:27:GLN:HE22	1.71	0.41
1:A:100:ASP:C	1:A:102:ASP:H	2.29	0.41
2:D:33:LEU:HD11	2:D:88:CYS:HB2	2.03	0.41
2:D:11:LEU:HD11	2:D:19:VAL:HG11	2.02	0.41
1:A:91:THR:C	1:A:92:VAL:HG23	2.46	0.40
2:B:54:LEU:HD21	2:B:60:SER:HA	2.02	0.40
2:B:147:LYS:HE3	2:B:147:LYS:HB2	1.60	0.40
2:B:188:ARG:NH2	3:B:309:HOH:O	2.43	0.40
2:D:28:ASP:OD1	2:D:28:ASP:C	2.64	0.40
1:A:136:ALA:H	2:B:213:GLU:CD	2.27	0.40
2:B:38:GLN:O	2:B:84:ALA:HB1	2.22	0.40
2:B:150:ILE:HD11	2:B:179:LEU:HD21	2.02	0.40
1:A:36:HIS:CD2	1:A:107:PHE:CE1	3.09	0.40
1:A:68:VAL:HG22	1:A:83:MET:CG	2.39	0.40
1:A:188:VAL:O	1:A:188:VAL:HG13	2.22	0.40
2:D:170:ASP:OD1	2:D:172:THR:HG23	2.22	0.40
1:A:2:GLN:H	1:A:2:GLN:CD	2.29	0.40
2:B:146:VAL:HG12	2:B:147:LYS:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:SER:OG	2:D:76:ASN:ND2[4_455]	2.15	0.05

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	225/233 (97%)	198 (88%)	23 (10%)	4 (2%)	6 12
1	C	225/233 (97%)	205 (91%)	14 (6%)	6 (3%)	4 6
2	B	214/216 (99%)	205 (96%)	6 (3%)	3 (1%)	9 17
2	D	214/216 (99%)	190 (89%)	20 (9%)	4 (2%)	6 11
All	All	878/898 (98%)	798 (91%)	63 (7%)	17 (2%)	6 11

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	TYR
1	A	221	ASP
1	A	222	ALA
1	C	85	SER
1	C	224	ALA
2	D	7	THR
2	D	26	SER
2	D	27	GLN
1	C	65	MET
1	C	90	ASP
2	B	211	ARG
1	C	102	ASP
2	D	69	ILE
1	A	86	LEU
2	B	212	ASN
2	B	68	GLY

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Mol	Chain	Res	Type
1	C	138	GLN

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	A	190/200 (95%)	182 (96%)	8 (4%)	26 52
1	C	194/200 (97%)	179 (92%)	15 (8%)	12 25
2	B	194/194 (100%)	185 (95%)	9 (5%)	24 48
2	D	194/194 (100%)	185 (95%)	9 (5%)	24 48
All	All	772/788 (98%)	731 (95%)	41 (5%)	20 42

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

Mol	Chain	Res	Type
1	A	18	SER
1	A	22	THR
1	A	31	THR
1	A	59	ASN
1	A	115	THR
1	A	154	PRO
1	A	156	PRO
1	A	218	VAL
2	B	33	LEU
2	B	97	THR
2	B	149	LYS
2	B	153	SER
2	B	181	LEU
2	B	199	LYS
2	B	200	THR
2	B	201	SER
2	B	213	GLU
1	C	8	SER
1	C	16	SER
1	C	25	VAL

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Mol	Chain	Res	Type
1	C	44	LYS
1	C	47	GLU
1	C	57	SER
1	C	66	SER
1	C	87	GLN
1	C	92	VAL
1	C	147	CYS
1	C	168	SER
1	C	176	VAL
1	C	179	SER
1	C	180	ASP
1	C	202	CYS
2	D	5	THR
2	D	7	THR
2	D	21	ILE
2	D	63	SER
2	D	79	GLU
2	D	201	SER
2	D	203	SER
2	D	208	SER
2	D	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
2	B	38	GLN
2	B	89	GLN
2	B	145	ASN
2	B	189	HIS
2	B	190	ASN
1	C	78	GLN
2	D	76	ASN
2	D	137	ASN
2	D	138	ASN
2	D	156	GLN

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 oligosaccharides 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	131:LEU	C	132:ALA	N	1.04

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	227/233 (97%)	0.23	16 (7%)	22	20	28, 47, 94, 124	0
1	C	227/233 (97%)	0.31	20 (8%)	15	14	28, 57, 94, 118	0
2	B	216/216 (100%)	-0.24	6 (2%)	55	50	28, 41, 65, 115	0
2	D	216/216 (100%)	0.28	10 (4%)	37	33	34, 59, 93, 108	0
All	All	886/898 (98%)	0.15	52 (5%)	28	24	28, 50, 92, 124	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	TYR	7.1
1	A	226	PRO	4.6
1	C	64	LEU	4.2
1	A	227	CYS	4.2
1	A	224	ALA	4.0
1	A	103	TYR	3.9
1	C	226	PRO	3.7
2	B	215	SER	3.7
1	C	224	ALA	3.6
2	D	214	CYS	3.5
1	A	135	SER	3.5
2	B	214	CYS	3.5
1	C	227	CYS	3.5
2	B	212	ASN	3.4
2	D	216	ASN	3.4
1	C	85	SER	3.3
2	B	216	ASN	3.3
1	C	222	ALA	3.2
1	C	103	TYR	3.1
1	A	222	ALA	3.0
2	D	15	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	211	ARG	2.9
2	D	215	SER	2.8
1	A	42	PRO	2.8
2	D	27	GLN	2.8
1	A	102	ASP	2.8
2	B	213	GLU	2.8
2	D	25	ALA	2.7
1	C	42	PRO	2.7
1	A	88	THR	2.6
1	C	84	ASN	2.6
2	D	212	ASN	2.6
1	C	65	MET	2.5
1	C	88	THR	2.5
1	A	104	ASP	2.5
1	A	64	LEU	2.4
1	A	1	ALA	2.4
1	A	137	ALA	2.4
1	C	63	ALA	2.4
1	C	1	ALA	2.4
1	C	89	ASP	2.3
1	C	86	LEU	2.3
1	C	91	THR	2.3
1	A	83	MET	2.2
2	D	94	LEU	2.2
1	C	66	SER	2.2
1	C	225	LYS	2.2
1	A	43	GLY	2.1
1	C	223	GLY	2.1
2	D	71	TYR	2.1
2	D	93	THR	2.0
1	C	101	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.