Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:56 pm BST

PDB ID : 2VLR
Title : The Structural Dynamics and Energetics of an Immunodominant T-cell Receptor are Programmed by its Vbeta Domain
Authors : Ishizuka, J.; Stewart-Jones, G.; van der Merwe, A.; Bell, J.; McMichael, A.; Jones, Y.
Deposited on : 2008-01-15
Resolution : 2.30 Å(reported)

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

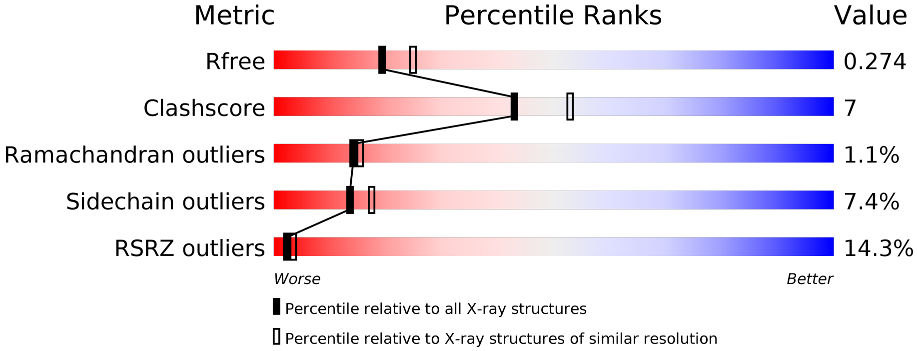
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

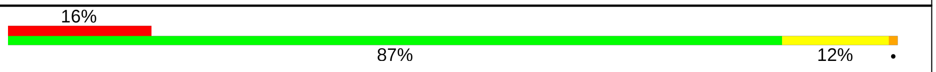
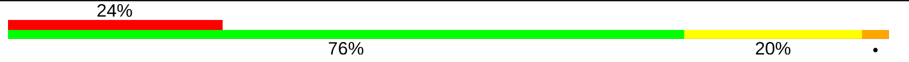
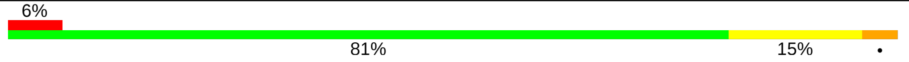
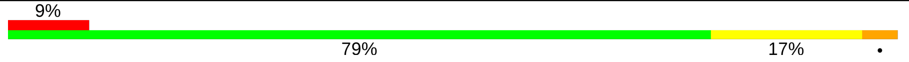
The reported resolution of this entry is 2.30 Å.

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	276	
1	F	276	
2	B	100	
2	G	100	
3	C	9	
3	H	9	

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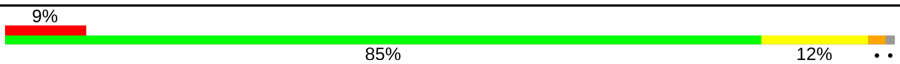
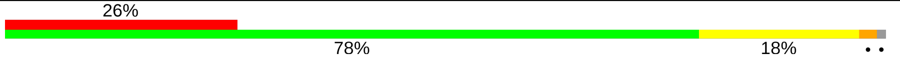
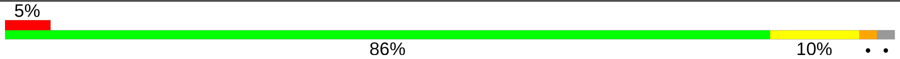
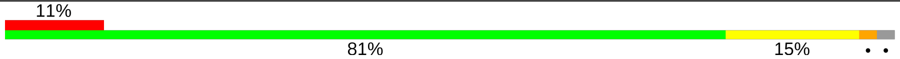
Mol	Chain	Length	Quality of chain
4	D	201	
4	I	201	
5	E	244	
5	J	244	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13819 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 HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	276	Total C N O S 2253 1408 410 426 9	1	0	0
1	F	276	Total C N O S 2253 1408 410 426 9	1	0	0

- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	100	Total C N O S 836 533 141 158 4	0	0	0
2	G	100	Total C N O S 836 533 141 158 4	0	0	0

- Molecule 3 is a protein called FLU MATRIX PEPTIDE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	9	Total C N O 68 49 9 10	0	0	0
3	H	9	Total C N O 68 49 9 10	0	0	0

- Molecule 4 is a protein called JM22 TCR ALPHA CHAIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	199	Total C N O S 1530 959 255 310 6	0	0	0
4	I	199	Total C N O S 1530 959 255 310 6	0	0	0

- Molecule 5 is a protein called JM22 TCR BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	240	1931	1218	334	374	5	0	0	0
5	J	240	1931	1218	334	374	5	0	0	0

- Molecule 6 is water.

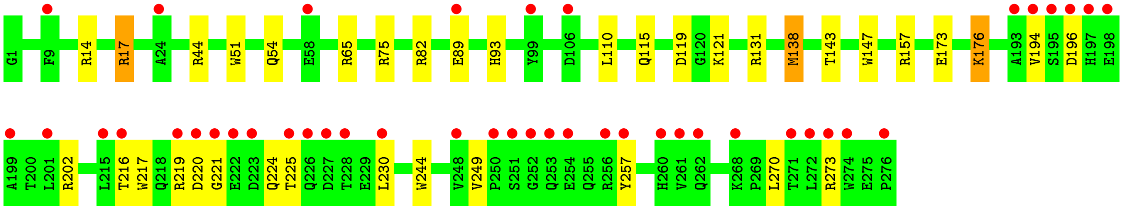
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	90	90	90	0	0
6	B	36	36	36	0	0
6	C	6	6	6	0	0
6	D	75	75	75	0	0
6	E	99	99	99	0	0
6	F	79	79	79	0	0
6	G	36	36	36	0	0
6	H	5	5	5	0	0
6	I	70	70	70	0	0
6	J	87	87	87	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

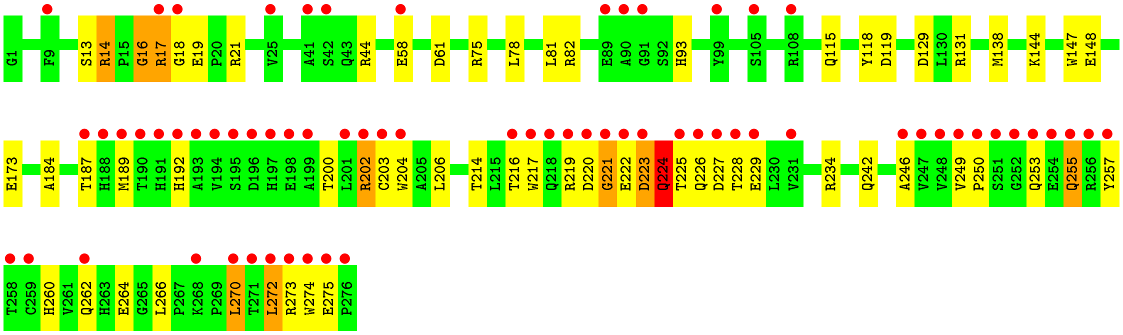
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

Chain A:



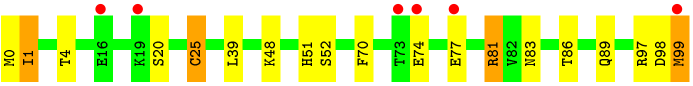
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

Chain F:



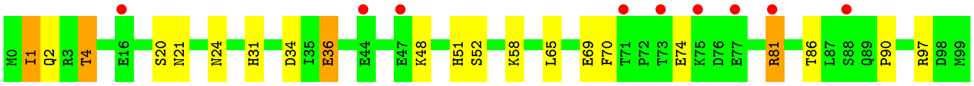
- Molecule 2: BETA-2-MICROGLOBULIN

Chain B:



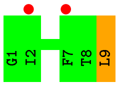
- Molecule 2: BETA-2-MICROGLOBULIN

Chain G:



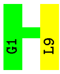
- Molecule 3: FLU MATRIX PEPTIDE

Chain C:



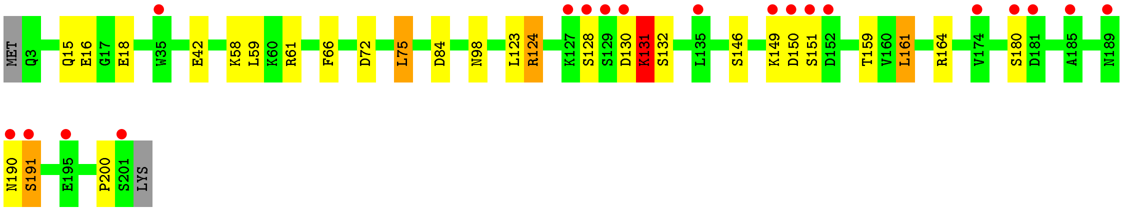
- Molecule 3: FLU MATRIX PEPTIDE

Chain H:



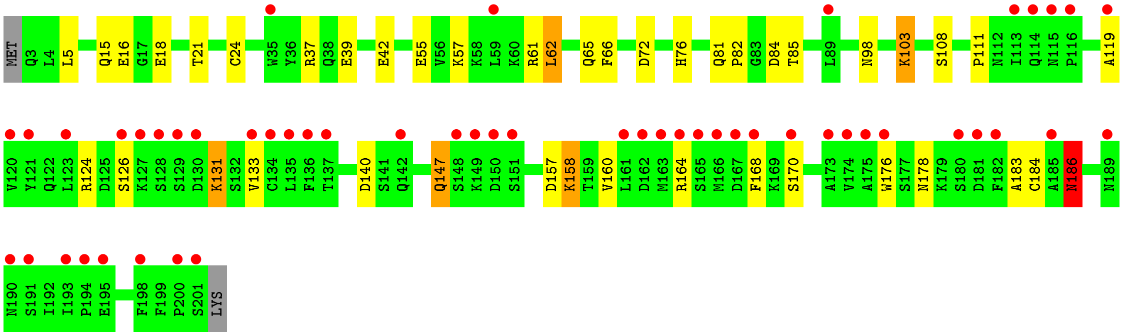
- Molecule 4: JM22 TCR ALPHA CHAIN

Chain D:



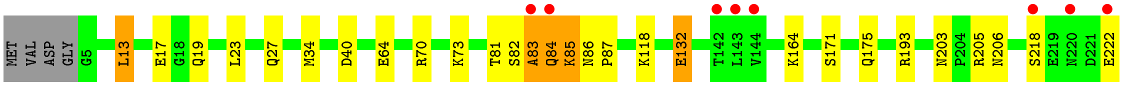
- Molecule 4: JM22 TCR ALPHA CHAIN

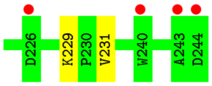
Chain I:



- Molecule 5: JM22 TCR BETA CHAIN

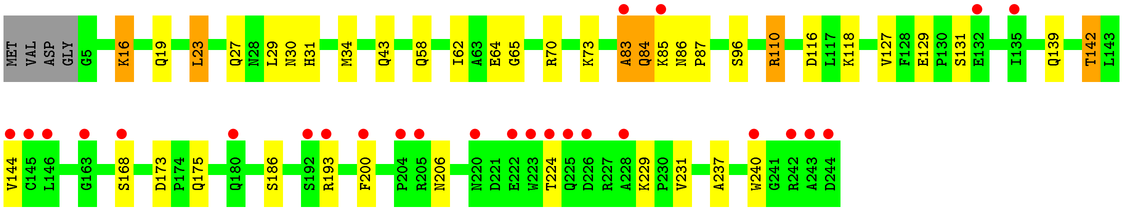
Chain E:





- Molecule 5: JM22 TCR BETA CHAIN

Chain J:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.62Å 95.52Å 122.05Å 110.29° 98.64° 93.59°	Depositor
Resolution (Å)	112.51 – 2.30 29.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (112.51-2.30) 97.5 (29.69-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.281 0.215 , 0.274	Depositor DCC
R_{free} test set	4402 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13819	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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 (i)

5.1 Standard geometry (i)

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	2.71	2/2319 (0.1%)	1.20	5/3149 (0.2%)
1	F	4.06	4/2319 (0.2%)	1.18	6/3149 (0.2%)
2	B	0.78	1/859 (0.1%)	0.72	0/1162
2	G	0.69	0/859	0.68	0/1162
3	C	1.30	0/69	1.03	1/92 (1.1%)
3	H	1.31	0/69	0.93	0/92
4	D	0.93	1/1560 (0.1%)	0.87	3/2113 (0.1%)
4	I	0.90	1/1560 (0.1%)	0.76	1/2113 (0.0%)
5	E	0.95	0/1984	0.82	4/2699 (0.1%)
5	J	0.83	0/1984	0.75	1/2699 (0.0%)
All	All	2.14	9/13582 (0.1%)	0.94	21/18430 (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	F	0	1
5	J	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	224	GLN	CA-CB	185.41	5.61	1.53
1	A	224	GLN	CA-CB	118.31	4.14	1.53
1	F	224	GLN	CB-CG	46.03	2.76	1.52
1	A	224	GLN	CB-CG	-39.50	0.46	1.52
4	I	158	LYS	CE-NZ	13.15	1.81	1.49
1	F	224	GLN	CD-OE1	12.90	1.52	1.24
2	B	25	CYS	CB-SG	6.04	1.92	1.82
1	F	224	GLN	CD-NE2	5.59	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	16	GLU	CG-CD	5.01	1.59	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	224	GLN	N-CA-CB	-45.82	28.13	110.60
1	A	224	GLN	CA-CB-CG	-43.14	18.49	113.40
1	A	224	GLN	N-CA-CB	-20.84	73.09	110.60
1	F	224	GLN	CB-CA-C	-12.99	84.42	110.40
1	A	224	GLN	CB-CA-C	-12.24	85.92	110.40
1	F	224	GLN	CA-CB-CG	10.71	136.95	113.40
4	D	161	LEU	CA-CB-CG	9.62	137.42	115.30
4	D	75	LEU	CA-CB-CG	7.77	133.17	115.30
1	F	18	GLY	N-CA-C	-6.79	96.13	113.10
1	A	44	ARG	NE-CZ-NH2	-6.59	117.00	120.30
5	E	40	ASP	CB-CG-OD1	6.07	123.76	118.30
5	E	23	LEU	CA-CB-CG	5.91	128.88	115.30
5	J	23	LEU	CA-CB-CG	5.80	128.65	115.30
5	E	13	LEU	CA-CB-CG	5.61	128.20	115.30
1	F	16	GLY	N-CA-C	5.59	127.09	113.10
1	F	129	ASP	CB-CG-OD1	5.41	123.17	118.30
4	I	62	LEU	CA-CB-CG	5.23	127.33	115.30
3	C	9	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	110	LEU	CA-CB-CG	5.19	127.24	115.30
5	E	13	LEU	CB-CG-CD1	-5.15	102.25	111.00
4	D	75	LEU	CB-CG-CD1	5.13	119.71	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	17	ARG	Peptide
5	J	84	GLN	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	2253	0	2103	17	1
1	F	2253	0	2103	37	2
2	B	836	0	803	13	2
2	G	836	0	803	13	1
3	C	68	0	75	2	0
3	H	68	0	75	1	0
4	D	1530	0	1480	16	0
4	I	1530	0	1480	26	0
5	E	1931	0	1829	24	0
5	J	1931	0	1829	32	0
6	A	90	0	0	7	0
6	B	36	0	0	2	0
6	C	6	0	0	0	0
6	D	75	0	0	1	0
6	E	99	0	0	5	0
6	F	79	0	0	9	0
6	G	36	0	0	2	0
6	H	5	0	0	0	0
6	I	70	0	0	7	0
6	J	87	0	0	7	0
All	All	13819	0	12580	175	3

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 (175) 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)
4:I:158:LYS:NZ	4:I:158:LYS:CE	1.81	1.41
2:G:81:ARG:HH11	2:G:81:ARG:HG2	0.94	1.09
1:A:17:ARG:NH1	6:A:2007:HOH:O	1.91	1.02
5:E:81:THR:O	5:E:83:ALA:N	1.96	0.98
2:G:81:ARG:NH1	2:G:81:ARG:HG2	1.73	0.95
5:E:86:ASN:HB3	6:E:2053:HOH:O	1.66	0.94
1:F:266:LEU:HD22	1:F:270:LEU:HD23	1.56	0.88
4:D:61:ARG:NH1	4:D:84:ASP:OD2	2.07	0.87
4:I:119:ALA:HB1	6:I:2052:HOH:O	1.74	0.86
5:E:84:GLN:NE2	5:E:85:LYS:H	1.73	0.86
5:J:84:GLN:O	5:J:86:ASN:N	2.07	0.85
1:A:17:ARG:NH2	6:A:2007:HOH:O	2.08	0.84
2:B:81:ARG:HH11	2:B:81:ARG:HG2	1.42	0.83
2:G:81:ARG:NH1	2:G:90:PRO:HB3	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:ARG:HH11	4:D:124:ARG:CG	1.93	0.82
5:E:84:GLN:HE21	5:E:85:LYS:H	1.27	0.81
1:F:216:THR:HA	6:F:2063:HOH:O	1.84	0.78
5:J:65:GLY:HA3	5:J:83:ALA:HA	1.63	0.78
2:G:81:ARG:HH11	2:G:81:ARG:CG	1.87	0.77
1:F:17:ARG:HB3	6:F:2005:HOH:O	1.84	0.76
2:B:4:THR:HG22	2:B:86:THR:OG1	1.86	0.76
1:F:217:TRP:HB2	6:F:2066:HOH:O	1.85	0.76
4:D:124:ARG:HG3	4:D:124:ARG:HH11	1.52	0.74
5:J:116:ASP:OD1	5:J:118:LYS:HG2	1.87	0.74
1:A:17:ARG:CZ	6:A:2007:HOH:O	2.25	0.74
5:E:86:ASN:OD1	6:E:2054:HOH:O	2.07	0.72
5:J:34:MET:HE3	5:J:70:ARG:NE	2.05	0.72
1:F:202:ARG:NH1	1:F:246:ALA:HB2	2.06	0.70
4:D:124:ARG:HD3	4:D:124:ARG:H	1.56	0.70
5:J:34:MET:HE2	5:J:70:ARG:NH2	2.06	0.69
4:I:61:ARG:NH1	4:I:84:ASP:OD2	2.24	0.69
4:I:103:LYS:HE3	6:J:2026:HOH:O	1.92	0.68
2:B:98:ASP:HB2	6:B:2036:HOH:O	1.93	0.68
5:J:142:THR:HG22	6:J:2065:HOH:O	1.93	0.67
2:G:2:GLN:HG2	6:G:2001:HOH:O	1.95	0.67
2:G:81:ARG:HH12	2:G:90:PRO:HB3	1.57	0.67
5:E:84:GLN:HE21	5:E:85:LYS:N	1.93	0.66
4:D:146:SER:H	4:D:191:SER:HB3	1.60	0.66
5:J:16:LYS:H	5:J:19:GLN:HE21	1.40	0.66
4:I:140:ASP:HA	6:I:2055:HOH:O	1.95	0.65
5:E:132:GLU:H	5:E:132:GLU:CD	2.01	0.64
1:F:187:THR:OG1	1:F:272:LEU:HD13	1.97	0.63
1:F:228:THR:HA	1:F:246:ALA:O	1.99	0.63
4:I:111:PRO:HG3	4:I:160:VAL:HG11	1.80	0.62
5:J:34:MET:HE2	5:J:70:ARG:HH21	1.65	0.62
5:J:34:MET:CE	5:J:70:ARG:NE	2.64	0.61
4:D:58:LYS:O	4:D:59:LEU:HD13	2.01	0.60
5:J:58:GLN:HG2	6:J:2028:HOH:O	2.01	0.60
4:D:61:ARG:HH12	4:D:84:ASP:CG	2.01	0.60
5:E:34:MET:HE3	5:E:70:ARG:NE	2.17	0.60
5:J:173:ASP:OD1	5:J:193:ARG:NH2	2.35	0.60
2:B:51:HIS:HD2	2:B:52:SER:O	1.86	0.59
4:D:15:GLN:O	4:D:18:GLU:HG3	2.02	0.59
4:I:131:LYS:HG3	6:I:2065:HOH:O	2.02	0.59
1:F:234:ARG:HE	1:F:242:GLN:HE21	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.84	0.59
4:D:131:LYS:HA	6:D:2059:HOH:O	2.02	0.59
2:B:74:GLU:HB2	6:B:2029:HOH:O	2.03	0.58
5:E:81:THR:C	5:E:83:ALA:N	2.56	0.58
5:J:34:MET:CE	5:J:70:ARG:HE	2.17	0.58
5:E:19:GLN:NE2	6:E:2008:HOH:O	2.36	0.58
2:B:1:ILE:O	2:B:1:ILE:CG2	2.51	0.58
4:I:158:LYS:NZ	4:I:158:LYS:CD	2.65	0.57
1:F:184:ALA:O	6:F:2052:HOH:O	2.17	0.57
1:F:229:GLU:HA	6:F:2068:HOH:O	2.04	0.56
4:I:81:GLN:HB3	4:I:82:PRO:HD2	1.87	0.56
1:A:65:ARG:NH1	6:A:2027:HOH:O	2.37	0.56
1:F:234:ARG:HE	1:F:242:GLN:NE2	2.02	0.56
4:I:61:ARG:HH12	4:I:84:ASP:CG	2.09	0.56
5:J:229:LYS:HG3	5:J:231:VAL:HG13	1.87	0.56
1:A:75:ARG:HD2	6:A:2010:HOH:O	2.06	0.55
4:I:183:ALA:O	4:I:186:ASN:ND2	2.39	0.55
1:F:14:ARG:NE	1:F:19:GLU:O	2.39	0.55
1:F:214:THR:HB	1:F:262:GLN:HB2	1.88	0.55
1:F:223:ASP:HA	1:F:224:GLN:HE21	1.72	0.55
4:I:15:GLN:O	4:I:18:GLU:HG3	2.06	0.55
5:J:84:GLN:C	5:J:86:ASN:H	2.00	0.55
4:D:124:ARG:CD	4:D:124:ARG:H	2.20	0.55
4:I:147:GLN:H	4:I:147:GLN:HE21	1.55	0.55
4:I:37:ARG:NH1	4:I:85:THR:O	2.40	0.54
5:J:34:MET:HE3	5:J:70:ARG:HE	1.72	0.54
2:B:81:ARG:CG	2:B:81:ARG:HH11	2.13	0.54
1:A:131:ARG:HE	1:A:157:ARG:NH1	2.05	0.54
4:I:119:ALA:CB	6:I:2052:HOH:O	2.43	0.53
5:J:86:ASN:N	5:J:87:PRO:CD	2.72	0.53
1:F:249:VAL:HB	1:F:250:PRO:HD2	1.91	0.53
5:E:229:LYS:HG3	5:E:231:VAL:HG13	1.91	0.52
1:F:260:HIS:HB2	6:F:2062:HOH:O	2.09	0.52
1:F:202:ARG:HD2	1:F:204:TRP:CD1	2.45	0.52
1:F:147:TRP:CZ2	3:H:9:LEU:HD23	2.45	0.52
1:F:93:HIS:HD2	1:F:119:ASP:OD2	1.92	0.52
5:J:34:MET:CE	5:J:73:LYS:O	2.59	0.51
1:F:192:HIS:O	1:F:200:THR:HB	2.11	0.51
4:I:55:GLU:OE1	4:I:57:LYS:HE3	2.10	0.51
4:D:123:LEU:O	4:D:132:SER:HB2	2.11	0.51
5:E:118:LYS:NZ	6:E:2068:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:86:ASN:N	5:J:87:PRO:HD2	2.26	0.50
5:E:132:GLU:N	5:E:132:GLU:CD	2.64	0.50
1:A:147:TRP:CZ2	3:C:9:LEU:HD23	2.46	0.50
6:A:2083:HOH:O	2:B:99:MET:HG2	2.10	0.50
2:G:51:HIS:HD2	2:G:52:SER:O	1.95	0.50
4:I:164:ARG:HG2	5:J:168:SER:HB2	1.93	0.49
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.94	0.49
1:F:13:SER:HB3	1:F:78:LEU:HD13	1.93	0.49
5:J:34:MET:HE1	5:J:73:LYS:O	2.13	0.49
4:D:124:ARG:HH11	4:D:124:ARG:HG2	1.75	0.49
4:I:126:SER:HB3	5:J:129:GLU:HG3	1.95	0.48
1:F:257:TYR:HB2	6:F:2074:HOH:O	2.12	0.48
2:G:31:HIS:ND1	6:G:2011:HOH:O	2.32	0.48
5:J:200:PHE:O	5:J:206:ASN:ND2	2.33	0.48
1:F:202:ARG:HH11	1:F:246:ALA:HB2	1.78	0.48
5:J:64:GLU:OE1	6:J:2039:HOH:O	2.20	0.47
2:B:1:ILE:O	2:B:1:ILE:HG22	2.14	0.47
5:E:84:GLN:HG3	5:E:85:LYS:N	2.28	0.47
1:A:121:LYS:HE3	1:A:121:LYS:HB2	1.65	0.47
4:D:159:THR:HB	5:E:171:SER:OG	2.14	0.47
2:B:4:THR:CG2	2:B:86:THR:OG1	2.61	0.47
4:I:147:GLN:H	4:I:147:GLN:NE2	2.12	0.47
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.50	0.47
5:E:84:GLN:HE21	5:E:84:GLN:HA	1.80	0.47
1:F:44:ARG:NH2	1:F:61:ASP:OD1	2.48	0.47
1:A:173:GLU:OE1	1:A:176:LYS:NZ	2.47	0.47
5:E:84:GLN:HE21	5:E:84:GLN:CA	2.28	0.47
4:I:168:PHE:HD2	6:I:2063:HOH:O	1.98	0.47
5:E:84:GLN:CG	5:E:85:LYS:N	2.78	0.46
5:E:34:MET:HE2	5:E:70:ARG:NH2	2.30	0.46
1:F:203:CYS:HA	6:F:2054:HOH:O	2.14	0.46
2:G:24:ASN:HB3	2:G:65:LEU:HD11	1.98	0.46
4:I:81:GLN:HB3	4:I:82:PRO:CD	2.46	0.46
5:J:139:GLN:HB2	6:J:2064:HOH:O	2.15	0.46
1:A:219:ARG:O	1:A:221:GLY:N	2.49	0.45
4:I:133:VAL:HG12	4:I:176:TRP:HB3	1.98	0.45
1:A:51:TRP:O	1:A:54:GLN:HG2	2.16	0.45
5:J:34:MET:HE2	5:J:70:ARG:CZ	2.46	0.45
4:I:157:ASP:HB3	6:I:2060:HOH:O	2.15	0.45
1:F:144:LYS:O	1:F:148:GLU:HG3	2.17	0.45
2:B:81:ARG:NH1	2:B:81:ARG:HG2	2.20	0.45

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
5:E:86:ASN:N	5:E:87:PRO:HD3	2.31	0.45
5:J:110:ARG:HD3	6:J:2061:HOH:O	2.17	0.45
4:D:124:ARG:HG3	4:D:124:ARG:NH1	2.24	0.44
2:B:81:ARG:CG	2:B:81:ARG:NH1	2.75	0.44
4:D:159:THR:HG23	6:E:2083:HOH:O	2.17	0.44
1:F:249:VAL:HB	1:F:250:PRO:CD	2.46	0.44
5:J:16:LYS:HB3	5:J:16:LYS:NZ	2.33	0.44
1:F:81:LEU:HD13	1:F:118:TYR:CD1	2.53	0.44
2:G:4:THR:HG23	2:G:86:THR:OG1	2.17	0.44
5:J:16:LYS:H	5:J:19:GLN:NE2	2.11	0.43
5:J:29:LEU:O	5:J:30:ASN:CB	2.66	0.43
2:G:1:ILE:CG2	2:G:1:ILE:O	2.67	0.43
1:F:274:TRP:CG	1:F:275:GLU:N	2.87	0.43
4:D:130:ASP:OD1	4:D:131:LYS:N	2.43	0.43
1:F:14:ARG:NH1	1:F:21:ARG:HB2	2.34	0.42
4:I:16:GLU:HG2	6:I:2008:HOH:O	2.18	0.42
5:E:34:MET:CE	5:E:73:LYS:O	2.66	0.42
2:G:4:THR:CG2	2:G:86:THR:OG1	2.66	0.42
5:J:31:HIS:HB3	5:J:96:SER:O	2.19	0.42
5:E:203:ASN:HB3	5:E:206:ASN:ND2	2.34	0.42
1:F:202:ARG:HB2	1:F:202:ARG:HH11	1.83	0.42
4:I:5:LEU:HD22	4:I:24:CYS:SG	2.60	0.42
5:J:127:VAL:HG23	5:J:237:ALA:HB3	2.01	0.42
5:J:144:VAL:CG2	6:J:2065:HOH:O	2.67	0.41
1:F:202:ARG:HB2	1:F:202:ARG:NH1	2.36	0.41
1:A:249:VAL:HG22	6:A:2077:HOH:O	2.20	0.41
5:E:34:MET:HE3	5:E:70:ARG:CZ	2.50	0.41
2:G:21:ASN:O	2:G:69:GLU:HG3	2.20	0.41
1:F:131:ARG:CZ	1:F:131:ARG:HB2	2.51	0.41
1:A:217:TRP:CZ3	1:A:257:TYR:HB3	2.56	0.41
1:A:176:LYS:NZ	1:A:176:LYS:HB3	2.36	0.41
1:A:143:THR:HG21	3:C:9:LEU:HD22	2.03	0.40
1:F:219:ARG:O	1:F:221:GLY:N	2.55	0.40
1:F:255:GLN:HG3	1:F:255:GLN:H	1.65	0.40
5:E:34:MET:HE2	5:E:73:LYS:O	2.21	0.40
1:F:189:MET:HA	6:F:2058:HOH:O	2.20	0.40
1:F:206:LEU:HD23	1:F:242:GLN:HB3	2.03	0.40
4:I:21:THR:OG1	4:I:76:HIS:HD2	2.05	0.40

All (3) 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)
1:A:138:MET:SD	2:G:36:GLU:OE2[1_544]	1.67	0.53
2:B:81:ARG:NH2	1:F:138:MET:SD[1_444]	2.05	0.15
2:B:81:ARG:CZ	1:F:138:MET:SD[1_444]	2.06	0.14

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	274/276 (99%)	258 (94%)	15 (6%)	1 (0%)	34	42
1	F	274/276 (99%)	252 (92%)	15 (6%)	7 (3%)	5	4
2	B	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
2	G	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	15	17
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	197/201 (98%)	190 (96%)	5 (2%)	2 (1%)	15	17
4	I	197/201 (98%)	177 (90%)	17 (9%)	3 (2%)	10	10
5	E	238/244 (98%)	229 (96%)	7 (3%)	2 (1%)	19	23
5	J	238/244 (98%)	222 (93%)	14 (6%)	2 (1%)	19	23
All	All	1628/1660 (98%)	1526 (94%)	84 (5%)	18 (1%)	14	15

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	82	SER
5	E	83	ALA
1	F	224	GLN
5	J	83	ALA
5	J	85	LYS
4	D	131	LYS
1	F	16	GLY

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Mol	Chain	Res	Type
1	F	220	ASP
1	F	222	GLU
1	F	226	GLN
1	A	220	ASP
4	I	186	ASN
1	F	223	ASP
2	G	97	ARG
4	I	131	LYS
4	I	184	CYS
4	D	200	PRO
1	F	221	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/232 (100%)	218 (94%)	14 (6%)	19	26
1	F	232/232 (100%)	216 (93%)	16 (7%)	15	20
2	B	95/95 (100%)	84 (88%)	11 (12%)	5	6
2	G	95/95 (100%)	85 (90%)	10 (10%)	7	8
3	C	7/7 (100%)	7 (100%)	0	100	100
3	H	7/7 (100%)	7 (100%)	0	100	100
4	D	175/177 (99%)	159 (91%)	16 (9%)	9	11
4	I	175/177 (99%)	161 (92%)	14 (8%)	12	15
5	E	211/214 (99%)	198 (94%)	13 (6%)	18	25
5	J	211/214 (99%)	199 (94%)	12 (6%)	20	28
All	All	1440/1450 (99%)	1334 (93%)	106 (7%)	13	17

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	ARG

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Mol	Chain	Res	Type
1	A	82	ARG
1	A	89	GLU
1	A	115	GLN
1	A	138	MET
1	A	176	LYS
1	A	194	VAL
1	A	196	ASP
1	A	216	THR
1	A	225	THR
1	A	230	LEU
1	A	270	LEU
1	A	273	ARG
2	B	0	MET
2	B	1	ILE
2	B	20	SER
2	B	48	LYS
2	B	70	PHE
2	B	77	GLU
2	B	81	ARG
2	B	83	ASN
2	B	89	GLN
2	B	97	ARG
2	B	99	MET
4	D	42	GLU
4	D	66	PHE
4	D	72	ASP
4	D	75	LEU
4	D	98	ASN
4	D	124	ARG
4	D	128	SER
4	D	131	LYS
4	D	149	LYS
4	D	150	ASP
4	D	151	SER
4	D	161	LEU
4	D	164	ARG
4	D	180	SER
4	D	190	ASN
4	D	191	SER
5	E	13	LEU
5	E	17	GLU
5	E	27	GLN

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Mol	Chain	Res	Type
5	E	64	GLU
5	E	84	GLN
5	E	85	LYS
5	E	132	GLU
5	E	164	LYS
5	E	175	GLN
5	E	193	ARG
5	E	205	ARG
5	E	218	SER
5	E	222	GLU
1	F	14	ARG
1	F	58	GLU
1	F	75	ARG
1	F	82	ARG
1	F	115	GLN
1	F	173	GLU
1	F	202	ARG
1	F	224	GLN
1	F	225	THR
1	F	227	ASP
1	F	253	GLN
1	F	255	GLN
1	F	264	GLU
1	F	270	LEU
1	F	272	LEU
1	F	273	ARG
2	G	1	ILE
2	G	4	THR
2	G	20	SER
2	G	34	ASP
2	G	36	GLU
2	G	48	LYS
2	G	58	LYS
2	G	70	PHE
2	G	74	GLU
2	G	81	ARG
4	I	39	GLU
4	I	42	GLU
4	I	62	LEU
4	I	65	GLN
4	I	66	PHE
4	I	72	ASP

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Mol	Chain	Res	Type
4	I	98	ASN
4	I	103	LYS
4	I	108	SER
4	I	124	ARG
4	I	147	GLN
4	I	170	SER
4	I	178	ASN
4	I	186	ASN
5	J	16	LYS
5	J	23	LEU
5	J	27	GLN
5	J	43	GLN
5	J	62	ILE
5	J	110	ARG
5	J	131	SER
5	J	142	THR
5	J	175	GLN
5	J	186	SER
5	J	224	THR
5	J	240	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	242	GLN
2	B	2	GLN
2	B	51	HIS
2	B	83	ASN
4	D	76	HIS
4	D	98	ASN
4	D	114	GLN
4	D	142	GLN
5	E	27	GLN
5	E	43	GLN
5	E	84	GLN
5	E	175	GLN
5	E	233	GLN
1	F	3	HIS
1	F	72	GLN
1	F	93	HIS
1	F	115	GLN

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Mol	Chain	Res	Type
1	F	224	GLN
1	F	242	GLN
1	F	253	GLN
2	G	51	HIS
4	I	76	HIS
4	I	98	ASN
4	I	142	GLN
4	I	147	GLN
4	I	186	ASN
5	J	19	GLN
5	J	27	GLN
5	J	43	GLN
5	J	233	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 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	276/276 (100%)	0.85	43 (15%) 2 2	22, 35, 76, 95	1 (0%)
1	F	276/276 (100%)	1.53	67 (24%) 0 0	21, 38, 81, 94	1 (0%)
2	B	100/100 (100%)	0.36	6 (6%) 21 28	26, 40, 52, 65	0
2	G	100/100 (100%)	0.45	9 (9%) 9 12	26, 40, 54, 64	0
3	C	9/9 (100%)	1.59	2 (22%) 0 1	21, 22, 23, 23	0
3	H	9/9 (100%)	0.92	0 100 100	17, 22, 24, 24	0
4	D	199/201 (99%)	0.64	19 (9%) 8 11	18, 35, 57, 65	0
4	I	199/201 (99%)	1.26	52 (26%) 0 0	19, 36, 82, 84	0
5	E	240/244 (98%)	0.36	12 (5%) 28 35	20, 34, 51, 62	0
5	J	240/244 (98%)	0.63	26 (10%) 5 8	20, 42, 60, 67	0
All	All	1648/1660 (99%)	0.83	236 (14%) 2 3	17, 37, 77, 95	2 (0%)

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	220	ASP	11.8
1	F	190	THR	11.8
1	F	256	ARG	11.4
1	A	194	VAL	10.8
1	F	199	ALA	10.7
1	F	272	LEU	9.4
1	F	193	ALA	9.4
1	F	276	PRO	9.3
1	F	221	GLY	8.9
1	F	271	THR	8.9
1	F	196	ASP	8.3
1	F	252	GLY	8.1
1	F	249	VAL	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	196	ASP	8.1
1	A	276	PRO	8.0
1	F	273	ARG	7.8
1	A	199	ALA	7.6
1	F	226	GLN	7.6
1	A	197	HIS	7.4
1	F	275	GLU	7.3
1	F	258	THR	6.9
1	F	250	PRO	6.9
4	I	166	MET	6.7
1	F	195	SER	6.6
4	I	129	SER	6.5
4	D	129	SER	6.4
1	F	248	VAL	6.3
5	J	243	ALA	6.3
1	F	254	GLU	6.2
4	I	135	LEU	6.2
1	F	228	THR	5.9
1	A	222	GLU	5.9
1	A	193	ALA	5.9
1	A	195	SER	5.9
1	F	191	HIS	5.8
4	I	114	GLN	5.8
1	A	221	GLY	5.8
4	I	201	SER	5.7
1	F	274	TRP	5.6
4	D	180	SER	5.6
1	F	198	GLU	5.6
1	A	228	THR	5.5
4	I	149	LYS	5.5
4	I	133	VAL	5.5
1	F	201	LEU	5.4
1	F	246	ALA	5.4
1	F	192	HIS	5.4
5	J	224	THR	5.4
1	F	255	GLN	5.3
1	F	217	TRP	5.2
1	F	225	THR	5.2
1	F	259	CYS	5.1
1	A	274	TRP	5.1
4	D	190	ASN	4.9
1	F	251	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	197	HIS	4.9
5	E	244	ASP	4.9
4	I	181	ASP	4.9
1	A	225	THR	4.9
1	F	247	VAL	4.8
4	D	128	SER	4.7
1	F	229	GLU	4.7
4	I	134	CYS	4.6
5	J	204	PRO	4.6
1	A	227	ASP	4.6
5	J	240	TRP	4.6
4	I	180	SER	4.5
4	I	167	ASP	4.5
1	F	189	MET	4.5
1	A	223	ASP	4.5
1	F	219	ARG	4.5
1	F	194	VAL	4.4
5	J	220	ASN	4.4
4	I	130	ASP	4.3
4	I	126	SER	4.3
4	I	174	VAL	4.2
5	E	220	ASN	4.2
1	F	257	TYR	4.2
5	J	200	PHE	4.1
1	F	204	TRP	4.1
4	D	201	SER	4.1
4	I	185	ALA	4.1
5	J	144	VAL	4.1
1	A	250	PRO	4.1
4	D	151	SER	4.0
1	F	253	GLN	4.0
4	D	130	ASP	4.0
4	I	164	ARG	3.9
4	I	194	PRO	3.9
1	F	17	ARG	3.8
1	A	273	ARG	3.8
1	F	216	THR	3.8
4	I	151	SER	3.8
1	A	268	LYS	3.7
4	D	149	LYS	3.7
5	J	163	GLY	3.7
5	J	132	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
5	E	240	TRP	3.6
4	I	123	LEU	3.6
5	J	85	LYS	3.6
2	B	99	MET	3.5
1	A	254	GLU	3.5
2	B	77	GLU	3.4
4	I	189	ASN	3.4
1	A	257	TYR	3.4
4	D	152	ASP	3.3
5	J	244	ASP	3.3
2	G	73	THR	3.3
1	A	201	LEU	3.3
4	I	173	ALA	3.3
4	D	127	LYS	3.3
1	F	222	GLU	3.3
1	A	260	HIS	3.2
5	J	242	ARG	3.2
4	I	168	PHE	3.2
2	G	77	GLU	3.2
1	F	270	LEU	3.2
5	E	222	GLU	3.2
5	J	222	GLU	3.2
4	I	182	PHE	3.2
1	A	251	SER	3.1
1	F	188	HIS	3.1
5	E	144	VAL	3.1
4	I	175	ALA	3.0
2	G	81	ARG	3.0
5	E	226	ASP	3.0
4	I	150	ASP	3.0
1	A	226	GLN	3.0
5	J	146	LEU	2.9
5	E	218	SER	2.9
5	E	243	ALA	2.9
1	F	187	THR	2.9
4	I	198	PHE	2.9
1	F	58	GLU	2.9
5	E	143	LEU	2.9
1	A	252	GLY	2.9
1	F	202	ARG	2.9
4	D	181	ASP	2.9
4	I	193	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
4	I	165	SER	2.8
1	A	272	LEU	2.8
4	I	163	MET	2.8
1	F	90	ALA	2.8
1	A	253	GLN	2.8
1	F	262	GLN	2.8
5	J	135	ILE	2.8
4	D	135	LEU	2.8
1	F	231	VAL	2.8
1	A	215	LEU	2.7
1	A	219	ARG	2.7
1	A	256	ARG	2.7
5	J	205	ARG	2.7
1	F	203	CYS	2.7
4	D	185	ALA	2.7
1	F	99	TYR	2.7
4	I	191	SER	2.7
4	I	137	THR	2.7
2	G	88	SER	2.6
1	A	261	VAL	2.6
1	F	223	ASP	2.6
2	B	16	GLU	2.6
1	F	9	PHE	2.6
4	I	127	LYS	2.6
2	G	47	GLU	2.6
1	F	268	LYS	2.6
1	A	220	ASP	2.6
1	F	227	ASP	2.6
4	I	195	GLU	2.5
2	B	19	LYS	2.5
4	I	136	PHE	2.5
1	F	105	SER	2.5
1	F	89	GLU	2.5
1	A	262	GLN	2.5
5	J	225	GLN	2.5
4	I	128	SER	2.5
5	J	145	CYS	2.5
1	F	108	ARG	2.4
4	D	35	TRP	2.4
4	I	120	VAL	2.4
1	A	248	VAL	2.4
4	I	176	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	41	ALA	2.4
4	I	119	ALA	2.4
5	J	223	TRP	2.4
2	G	75	LYS	2.4
4	I	116	PRO	2.4
2	G	71	THR	2.4
5	J	193	ARG	2.4
1	A	230	LEU	2.4
2	G	16	GLU	2.3
5	E	142	THR	2.3
5	J	226	ASP	2.3
2	G	44	GLU	2.3
4	I	162	ASP	2.3
4	I	161	LEU	2.3
1	A	106	ASP	2.3
1	A	198	GLU	2.2
4	D	174	VAL	2.2
3	C	2	ILE	2.2
5	E	83	ALA	2.2
4	I	89	LEU	2.2
4	I	115	ASN	2.2
1	A	58	GLU	2.2
4	D	191	SER	2.2
4	I	35	TRP	2.2
1	F	18	GLY	2.2
4	I	200	PRO	2.2
5	J	168	SER	2.2
4	D	150	ASP	2.2
4	I	113	ILE	2.2
4	I	121	TYR	2.2
4	D	189	ASN	2.2
1	A	216	THR	2.2
5	J	192	SER	2.2
5	J	180	GLN	2.2
3	C	7	PHE	2.1
1	A	9	PHE	2.1
4	I	59	LEU	2.1
4	I	190	ASN	2.1
1	F	218	GLN	2.1
1	F	91	GLY	2.1
4	I	142	GLN	2.1
2	B	74	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	24	ALA	2.1
5	J	228	ALA	2.1
1	A	89	GLU	2.0
2	B	73	THR	2.0
4	D	195	GLU	2.0
5	E	84	GLN	2.0
5	J	83	ALA	2.0
1	F	25	VAL	2.0
1	A	99	TYR	2.0
1	A	271	THR	2.0
1	F	42	SER	2.0
4	I	148	SER	2.0
4	I	170	SER	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 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.