Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2016 – 02:56 PM EDT

PDB ID	:	5CDD
Title	:	Crystal Structure of Israel acute Paralysis Virus Pentamer
Authors	:	Mullapudi, E.; Plevka, P.
Deposited on	:	2015-07-03
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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 2.70 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
Clashscore		17
Ramachandran outliers		0.7%
Sidechain outliers		2.7%
RSRZ outliers		63.6%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
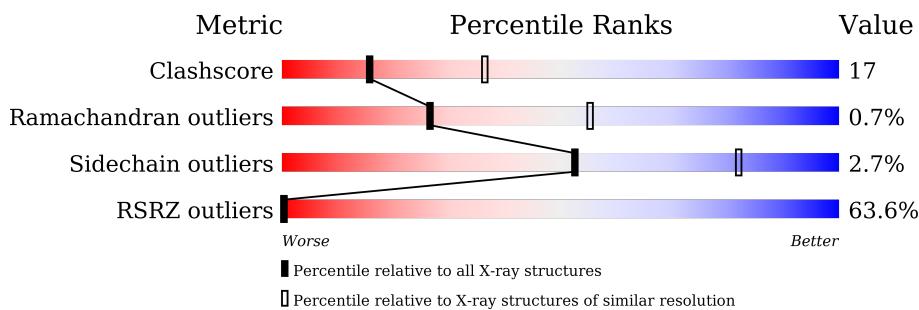
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	208	51% / 71% 26% ··
2	B	301	66% / 69% 30% ·
3	C	200	73% / 57% 39% 5%
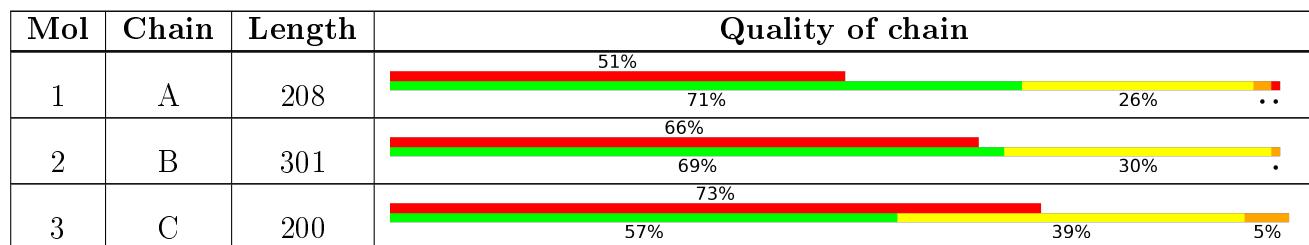
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5617 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 Structural polyprotein, VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1682	1065	286	324	7			

- Molecule 2 is a protein called Structural polyprotein, VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	301	Total	C	N	O	S	0	0	0
			2345	1500	386	446	13			

- Molecule 3 is a protein called Structural polyprotein, VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	200	Total	C	N	O	S	0	0	0
			1577	1012	257	303	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	87	ALA	ASN	conflict	UNP D1FK67

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	1	Total	O	0	0
			1	1		
4	C	2	Total	O	0	0
			2	2		

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

- Molecule 1: Structural polyprotein, VP1
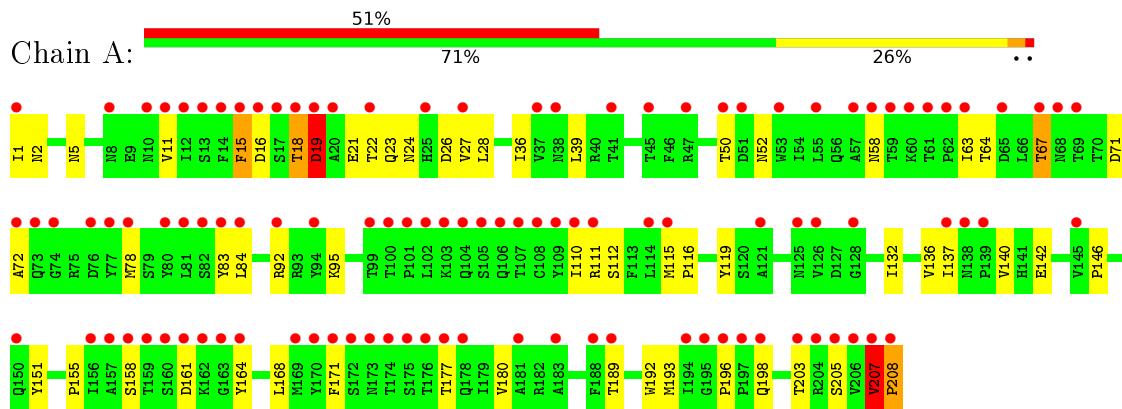
- Molecule 2: Structural polyprotein, VP3
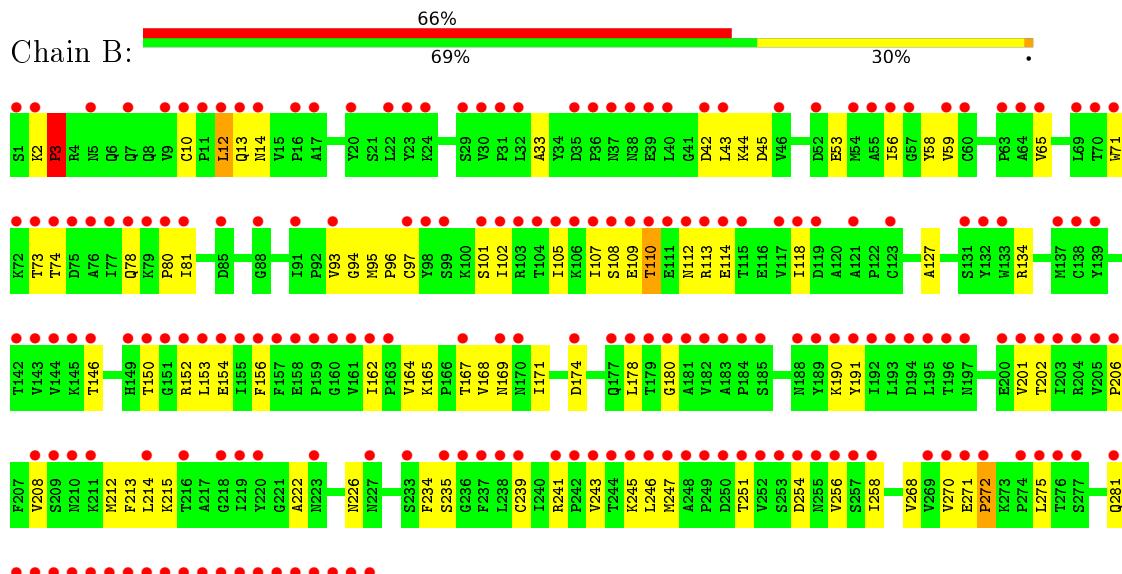
- Molecule 3: Structural polyprotein, VP2
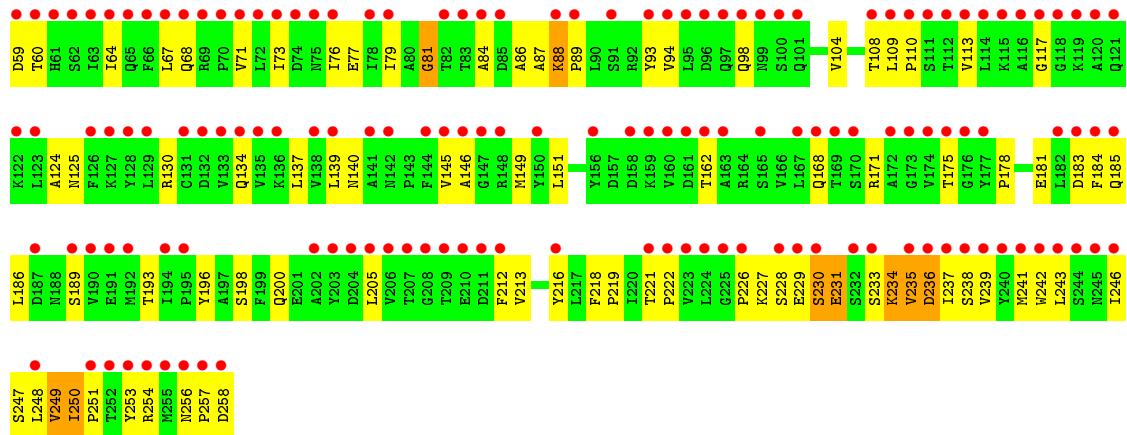
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.18Å 274.25Å 288.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 2.70 48.77 – 1.23	Depositor EDS
% Data completeness (in resolution range)	98.7 (70.00-2.70) 11.4 (48.77-1.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 1.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.251 0.525 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	1.6	Xtriage
Anisotropy	1.986	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.94 , 1768.4	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o,F_c correlation	0.24	EDS
Total number of atoms	5617	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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	A	0.45	3/1724 (0.2%)	0.75	7/2345 (0.3%)
2	B	0.33	1/2408 (0.0%)	0.60	0/3298
3	C	1.12	20/1612 (1.2%)	0.84	10/2198 (0.5%)
All	All	0.68	24/5744 (0.4%)	0.72	17/7841 (0.2%)

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	A	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	231	GLU	CD-OE1	-16.63	1.07	1.25
3	C	249	VAL	C-O	-14.45	0.95	1.23
3	C	250	ILE	C-O	-11.29	1.01	1.23
3	C	229	GLU	C-O	-10.06	1.04	1.23
3	C	251	PRO	C-O	-9.67	1.03	1.23
3	C	231	GLU	CD-OE2	-9.20	1.15	1.25
3	C	251	PRO	CA-C	-8.79	1.35	1.52
3	C	249	VAL	CB-CG1	-8.79	1.34	1.52
3	C	231	GLU	C-O	-8.70	1.06	1.23
3	C	229	GLU	CA-C	-8.40	1.31	1.52
3	C	230	SER	CB-OG	-8.29	1.31	1.42
3	C	229	GLU	CA-CB	-8.20	1.35	1.53
1	A	208	PRO	N-CD	7.85	1.58	1.47
3	C	230	SER	C-O	-7.67	1.08	1.23
3	C	249	VAL	N-CA	-7.08	1.32	1.46
3	C	229	GLU	CG-CD	-6.92	1.41	1.51
1	A	208	PRO	CA-C	-6.85	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	249	VAL	CB-CG2	-6.50	1.39	1.52
3	C	251	PRO	CA-CB	-6.12	1.41	1.53
2	B	3	PRO	N-CD	5.90	1.56	1.47
3	C	230	SER	CA-CB	-5.84	1.44	1.52
3	C	251	PRO	CG-CD	-5.31	1.33	1.50
1	A	208	PRO	CA-CB	-5.30	1.43	1.53
3	C	229	GLU	CD-OE1	-5.06	1.20	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	VAL	C-N-CD	-13.94	89.94	120.60
3	C	251	PRO	CA-N-CD	-9.59	98.07	111.50
1	A	208	PRO	CA-N-CD	-9.46	98.26	111.50
3	C	229	GLU	CB-CA-C	-8.85	92.69	110.40
1	A	207	VAL	CB-CA-C	-8.74	94.80	111.40
3	C	249	VAL	CG1-CB-CG2	-8.29	97.63	110.90
3	C	230	SER	CB-CA-C	-7.31	96.22	110.10
1	A	208	PRO	N-CA-CB	6.93	111.62	103.30
1	A	208	PRO	N-CD-CG	-6.50	93.44	103.20
1	A	19	ASP	N-CA-C	-6.08	94.59	111.00
3	C	81	GLY	N-CA-C	-5.82	98.54	113.10
1	A	16	ASP	N-CA-C	-5.82	95.30	111.00
3	C	249	VAL	CB-CA-C	-5.69	100.59	111.40
3	C	250	ILE	C-N-CD	5.69	140.34	128.40
3	C	236	ASP	O-C-N	-5.28	114.25	122.70
3	C	249	VAL	CA-CB-CG2	5.13	118.60	110.90
3	C	229	GLU	N-CA-CB	5.12	119.82	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	VAL	Mainchain

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	1682	0	1624	72	0
2	B	2345	0	2308	91	0
3	C	1577	0	1575	69	0
4	A	10	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
All	All	5617	0	5507	190	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 17.

All (190) 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:A:207:VAL:HB	1:A:208:PRO:CD	1.74	1.14
1:A:207:VAL:HB	1:A:208:PRO:HD3	1.18	1.11
2:B:65:VAL:H	3:C:175:THR:HG21	1.27	0.98
1:A:5:ASN:ND2	3:C:181:GLU:H	1.62	0.96
1:A:5:ASN:HD21	3:C:181:GLU:N	1.64	0.96
2:B:2:LYS:HB2	2:B:3:PRO:CD	1.98	0.94
1:A:207:VAL:O	1:A:208:PRO:C	1.96	0.93
1:A:27:VAL:CG1	2:B:212:MET:HB3	2.00	0.91
2:B:2:LYS:HB2	2:B:3:PRO:HD3	1.56	0.88
3:C:235:VAL:HG12	3:C:236:ASP:N	1.91	0.83
3:C:139:LEU:HD21	3:C:184:PHE:HA	1.61	0.82
2:B:107:ILE:HD11	2:B:113:ARG:HB2	1.62	0.82
2:B:165:LYS:HE3	2:B:174:ASP:HA	1.60	0.81
1:A:2:ASN:HD21	1:A:5:ASN:HD22	1.26	0.80
1:A:24:ASN:HD22	2:B:134:ARG:HE	1.29	0.79
1:A:207:VAL:CB	1:A:208:PRO:CD	2.57	0.79
1:A:27:VAL:HG13	2:B:212:MET:HB3	1.66	0.78
1:A:5:ASN:HD21	3:C:181:GLU:H	0.81	0.76
1:A:23:GLN:O	1:A:27:VAL:HG23	1.84	0.75
3:C:130:ARG:HB3	3:C:247:SER:HB3	1.67	0.75
2:B:12:LEU:HD22	2:B:13:GLN:H	1.50	0.74
1:A:24:ASN:ND2	2:B:134:ARG:HE	1.85	0.74
1:A:1:ILE:HG23	3:C:178:PRO:HA	1.69	0.74
3:C:76:ILE:O	3:C:236:ASP:OD1	2.06	0.73
1:A:2:ASN:ND2	1:A:5:ASN:HD22	1.89	0.71
2:B:214:LEU:HD11	2:B:235:SER:HB3	1.73	0.71
3:C:77:GLU:CD	3:C:234:LYS:HD2	2.12	0.70
1:A:207:VAL:HG12	1:A:208:PRO:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:ASP:CG	3:C:60:THR:H	1.97	0.67
2:B:44:LYS:O	2:B:45:ASP:HB2	1.96	0.66
1:A:67:THR:HG23	1:A:71:ASP:OD2	1.95	0.66
1:A:2:ASN:HD21	1:A:5:ASN:ND2	1.94	0.64
2:B:71:TRP:HB3	2:B:256:VAL:HG23	1.80	0.64
1:A:11:VAL:HG22	2:B:202:THR:HB	1.80	0.63
1:A:27:VAL:HG11	2:B:212:MET:HB3	1.80	0.63
1:A:189:THR:HG21	2:B:43:LEU:HD21	1.79	0.63
1:A:198:GLN:HE22	3:C:94:VAL:H	1.47	0.63
2:B:150:THR:OG1	2:B:247:MET:HB2	1.98	0.63
1:A:136:VAL:HG13	1:A:137:ILE:HG23	1.81	0.63
1:A:155:PRO:HB2	1:A:158:SER:HB2	1.79	0.63
1:A:111:ARG:HD2	1:A:132:ILE:HB	1.81	0.62
3:C:77:GLU:HA	3:C:236:ASP:HA	1.81	0.62
2:B:134:ARG:HB3	2:B:268:VAL:CG2	2.29	0.62
3:C:84:ALA:C	3:C:86:ALA:H	2.00	0.62
3:C:235:VAL:CG1	3:C:236:ASP:N	2.59	0.61
2:B:154:GLU:HB2	2:B:243:VAL:HG23	1.83	0.60
2:B:65:VAL:H	3:C:175:THR:CG2	2.10	0.60
3:C:253:TYR:CE1	3:C:254:ARG:HG3	2.36	0.60
2:B:153:LEU:HD21	2:B:258:ILE:HD13	1.84	0.60
3:C:140:ASN:O	3:C:235:VAL:O	2.21	0.59
1:A:193:MET:CE	2:B:59:VAL:HG22	2.32	0.59
1:A:63:ILE:HG12	1:A:168:LEU:HB3	1.85	0.59
3:C:237:ILE:HG22	3:C:238:SER:N	2.18	0.58
2:B:167:THR:HG22	2:B:168:VAL:N	2.19	0.58
1:A:95:LYS:HG2	1:A:142:GLU:HG2	1.86	0.58
3:C:145:VAL:CG2	3:C:233:SER:HB3	2.34	0.58
1:A:146:PRO:HG2	2:B:33:ALA:HB2	1.86	0.58
3:C:64:ILE:HG23	3:C:246:ILE:HD12	1.86	0.58
1:A:36:ILE:HG22	2:B:56:ILE:HD11	1.86	0.58
2:B:154:GLU:HB2	2:B:243:VAL:CG2	2.34	0.57
1:A:161:ASP:HA	1:A:164:TYR:CD2	2.40	0.57
3:C:64:ILE:O	3:C:68:GLN:HG3	2.04	0.57
1:A:27:VAL:HG12	2:B:213:PHE:CE2	2.40	0.57
3:C:139:LEU:CD2	3:C:184:PHE:HA	2.35	0.56
1:A:207:VAL:CG1	1:A:208:PRO:N	2.63	0.56
3:C:73:ILE:HG13	3:C:241:MET:HB2	1.88	0.55
2:B:73:THR:HA	2:B:246:LEU:HB3	1.87	0.55
2:B:42:ASP:OD1	2:B:44:LYS:HB3	2.07	0.55
2:B:71:TRP:HB3	2:B:256:VAL:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:O	1:A:132:ILE:HA	2.08	0.54
3:C:227:LYS:O	3:C:228:SER:HB2	2.08	0.54
3:C:234:LYS:NZ	3:C:234:LYS:HB3	2.23	0.54
1:A:18:THR:HG22	1:A:19:ASP:OD1	2.07	0.53
3:C:109:LEU:HB2	3:C:213:VAL:HG13	1.90	0.53
3:C:235:VAL:HG12	3:C:236:ASP:H	1.69	0.53
3:C:87:ALA:O	3:C:89:PRO:HD3	2.09	0.53
1:A:50:THR:HG22	1:A:180:VAL:HB	1.91	0.53
3:C:198:SER:HB2	3:C:212:PHE:CD2	2.43	0.53
1:A:52:ASN:HB2	2:B:301:GLN:HG3	1.91	0.52
3:C:196:TYR:CZ	3:C:198:SER:HB3	2.44	0.52
1:A:19:ASP:OD1	1:A:19:ASP:N	2.42	0.52
1:A:27:VAL:HG12	2:B:213:PHE:CZ	2.43	0.52
2:B:288:THR:HG22	2:B:290:SER:H	1.73	0.52
2:B:97:CYS:SG	2:B:118:ILE:HG22	2.49	0.52
1:A:116:PRO:HB2	1:A:119:TYR:CD1	2.44	0.52
1:A:19:ASP:C	1:A:21:GLU:N	2.60	0.52
3:C:87:ALA:O	3:C:88:LYS:C	2.48	0.52
3:C:108:THR:O	3:C:108:THR:HG23	2.10	0.52
1:A:161:ASP:HA	1:A:164:TYR:CE2	2.45	0.51
3:C:124:ALA:O	3:C:125:ASN:HB2	2.09	0.51
1:A:58:ASN:HA	1:A:171:PHE:CE1	2.46	0.51
2:B:80:PRO:HD3	2:B:178:LEU:O	2.11	0.51
2:B:12:LEU:CD2	2:B:13:GLN:H	2.23	0.50
2:B:93:VAL:O	2:B:234:PHE:O	2.30	0.50
2:B:97:CYS:SG	2:B:118:ILE:CG2	3.01	0.49
3:C:237:ILE:HG22	3:C:238:SER:H	1.76	0.49
3:C:76:ILE:O	3:C:236:ASP:HA	2.12	0.49
1:A:64:THR:HA	1:A:67:THR:HB	1.95	0.49
1:A:151:TYR:CE1	3:C:200:GLN:HG2	2.47	0.49
2:B:171:ILE:HD12	2:B:222:ALA:HB1	1.94	0.49
3:C:257:PRO:O	3:C:258:ASP:OD1	2.30	0.49
1:A:78:MET:HE1	1:A:92:ARG:NH1	2.27	0.49
3:C:134:GLN:NE2	3:C:193:THR:OG1	2.46	0.49
3:C:137:LEU:O	3:C:189:SER:HA	2.12	0.49
2:B:162:ILE:O	2:B:164:VAL:HG13	2.12	0.49
3:C:183:ASP:HB3	3:C:186:LEU:HB2	1.94	0.48
2:B:2:LYS:CB	2:B:3:PRO:CD	2.81	0.48
2:B:102:ILE:HD11	2:B:169:ASN:O	2.13	0.48
2:B:2:LYS:HB2	2:B:3:PRO:HD2	1.92	0.47
2:B:2:LYS:CB	2:B:3:PRO:HD3	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:GLN:HB3	2:B:180:GLY:HA3	1.96	0.47
1:A:177:THR:HG23	1:A:177:THR:O	2.14	0.47
1:A:24:ASN:HB3	2:B:268:VAL:HG11	1.95	0.47
1:A:111:ARG:HD3	1:A:132:ILE:HD12	1.97	0.47
1:A:205:SER:HA	2:B:112:ASN:O	2.14	0.47
3:C:59:ASP:CG	3:C:60:THR:N	2.67	0.47
1:A:24:ASN:ND2	2:B:134:ARG:NE	2.60	0.47
2:B:288:THR:HG22	2:B:289:ALA:N	2.29	0.47
2:B:222:ALA:HA	2:B:226:ASN:O	2.14	0.47
1:A:83:TYR:CD2	2:B:282:VAL:HG21	2.50	0.47
3:C:110:PRO:O	3:C:113:VAL:HG12	2.15	0.47
2:B:146:THR:HA	3:C:185:GLN:HG2	1.97	0.46
3:C:248:LEU:C	3:C:249:VAL:HG13	2.34	0.46
1:A:39:LEU:HD12	2:B:59:VAL:HG21	1.97	0.46
2:B:234:PHE:O	2:B:235:SER:CB	2.64	0.46
3:C:64:ILE:HG23	3:C:246:ILE:HB	1.98	0.46
2:B:156:PHE:CE2	2:B:239:CYS:HB3	2.51	0.46
2:B:95:MET:N	2:B:96:PRO:CD	2.79	0.46
1:A:63:ILE:CG1	1:A:168:LEU:HB3	2.46	0.45
3:C:67:LEU:HB2	3:C:246:ILE:HD13	1.98	0.45
1:A:72:ALA:HB1	2:B:284:ARG:CZ	2.46	0.45
1:A:140:VAL:HG12	1:A:142:GLU:HG3	1.99	0.45
1:A:28:LEU:HD12	2:B:213:PHE:HZ	1.82	0.45
2:B:270:VAL:O	2:B:271:GLU:HB3	2.17	0.45
1:A:112:SER:HB2	1:A:168:LEU:HD11	1.99	0.45
1:A:19:ASP:C	1:A:21:GLU:H	2.21	0.44
2:B:156:PHE:CB	2:B:190:LYS:HB3	2.47	0.44
2:B:251:THR:O	3:C:226:PRO:HB3	2.18	0.44
1:A:1:ILE:O	1:A:1:ILE:HG23	2.17	0.44
1:A:19:ASP:O	1:A:21:GLU:N	2.51	0.44
1:A:50:THR:O	1:A:50:THR:HG23	2.17	0.44
2:B:108:SER:OG	2:B:110:THR:HG23	2.17	0.44
2:B:156:PHE:HB3	2:B:190:LYS:HB3	2.00	0.43
2:B:287:PRO:O	3:C:98:GLN:HG3	2.18	0.43
3:C:205:LEU:O	3:C:256:ASN:HB2	2.18	0.43
3:C:171:ARG:O	3:C:175:THR:HG22	2.18	0.43
2:B:81:ILE:HD11	2:B:153:LEU:HD11	2.01	0.43
2:B:191:TYR:CD2	2:B:201:VAL:HG21	2.53	0.43
3:C:151:LEU:HD12	3:C:216:TYR:O	2.19	0.43
3:C:236:ASP:C	3:C:237:ILE:HG13	2.39	0.43
1:A:27:VAL:HA	2:B:212:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:VAL:HG11	3:C:243:LEU:HD21	1.99	0.42
1:A:1:ILE:HG23	3:C:178:PRO:CA	2.46	0.42
1:A:208:PRO:HB2	2:B:112:ASN:HD21	1.85	0.42
1:A:84:LEU:CD2	1:A:196:PRO:HB3	2.48	0.42
3:C:162:THR:HG22	3:C:168:GLN:HG3	2.00	0.42
3:C:221:THR:HB	3:C:222:PRO:HD2	2.01	0.42
2:B:167:THR:CG2	2:B:168:VAL:N	2.82	0.42
3:C:79:ILE:HG22	3:C:81:GLY:H	1.83	0.42
2:B:154:GLU:HB3	2:B:241:ARG:O	2.19	0.42
2:B:208:VAL:HG23	2:B:208:VAL:O	2.19	0.42
3:C:71:VAL:HG11	3:C:117:GLY:HA3	2.00	0.42
2:B:101:SER:HB2	3:C:93:TYR:CE2	2.54	0.42
1:A:28:LEU:HD12	2:B:213:PHE:CZ	2.55	0.42
2:B:281:GLN:NE2	2:B:296:LEU:HG	2.34	0.42
2:B:80:PRO:HA	2:B:241:ARG:HG2	2.01	0.42
3:C:134:GLN:HB3	3:C:242:TRP:CE2	2.55	0.42
3:C:104:VAL:HG21	3:C:149:MET:CE	2.50	0.42
3:C:248:LEU:C	3:C:249:VAL:CG1	2.87	0.42
2:B:254:ASP:OD1	3:C:227:LYS:HE3	2.20	0.42
3:C:218:PHE:HA	3:C:219:PRO:HD3	1.83	0.41
1:A:15:PHE:CD2	2:B:206:PRO:HD2	2.55	0.41
2:B:73:THR:O	2:B:245:LYS:HE2	2.20	0.41
2:B:81:ILE:HD13	2:B:258:ILE:HD12	2.02	0.41
2:B:105:ILE:CG1	2:B:113:ARG:HB3	2.51	0.41
2:B:53:GLU:HA	2:B:58:TYR:CD2	2.56	0.41
2:B:146:THR:CG2	3:C:146:ALA:HB2	2.51	0.41
2:B:94:GLY:HA3	2:B:234:PHE:HD1	1.86	0.41
2:B:271:GLU:HG3	2:B:272:PRO:CD	2.51	0.41
2:B:152:ARG:HH11	2:B:152:ARG:HG2	1.86	0.41
3:C:84:ALA:C	3:C:86:ALA:N	2.69	0.41
1:A:203:THR:HA	2:B:114:GLU:O	2.21	0.41
2:B:12:LEU:HA	2:B:12:LEU:HD23	1.81	0.41
1:A:19:ASP:O	1:A:22:THR:N	2.53	0.40
3:C:137:LEU:HD22	3:C:239:VAL:HG22	2.04	0.40
3:C:236:ASP:OD1	3:C:237:ILE:N	2.51	0.40
1:A:27:VAL:CG1	2:B:213:PHE:CZ	3.04	0.40
2:B:215:LYS:HB3	2:B:275:LEU:CD2	2.51	0.40
1:A:146:PRO:CG	2:B:33:ALA:HB2	2.51	0.40
2:B:95:MET:CE	2:B:127:ALA:HB2	2.51	0.40

There are no symmetry-related clashes.

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	206/208 (99%)	185 (90%)	19 (9%)	2 (1%)	19	45
2	B	299/301 (99%)	268 (90%)	29 (10%)	2 (1%)	26	55
3	C	198/200 (99%)	180 (91%)	17 (9%)	1 (0%)	34	63
All	All	703/709 (99%)	633 (90%)	65 (9%)	5 (1%)	26	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	272	PRO
1	A	207	VAL
3	C	250	ILE
1	A	15	PHE
2	B	3	PRO

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	189/189 (100%)	183 (97%)	6 (3%)	46	77
2	B	263/263 (100%)	257 (98%)	6 (2%)	58	85
3	C	177/177 (100%)	172 (97%)	5 (3%)	51	81
All	All	629/629 (100%)	612 (97%)	17 (3%)	52	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	19	ASP
1	A	26	ASP
1	A	67	THR
1	A	115	MET
1	A	192	TRP
2	B	10	CYS
2	B	12	LEU
2	B	14	ASN
2	B	74	THR
2	B	109	GLU
2	B	110	THR
3	C	88	LYS
3	C	230	SER
3	C	231	GLU
3	C	234	LYS
3	C	235	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	24	ASN
1	A	131	HIS
1	A	141	HIS
1	A	198	GLN
2	B	13	GLN
2	B	187	ASN
2	B	255	ASN
2	B	281	GLN
3	C	97	GLN
3	C	134	GLN
3	C	188	ASN

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 carbohydrates 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 (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, 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	208/208 (100%)	3.70	107 (51%)	0	0	20, 34, 62, 80	0
2	B	301/301 (100%)	7.55	199 (66%)	0	0	24, 39, 69, 92	0
3	C	200/200 (100%)	6.82	145 (72%)	0	0	27, 42, 89, 102	0
All	All	709/709 (100%)	6.22	451 (63%)	0	0	20, 39, 72, 102	0

All (451) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	105	ILE	72.3
2	B	110	THR	67.1
2	B	108	SER	63.3
2	B	112	ASN	57.4
2	B	246	LEU	51.7
1	A	208	PRO	44.7
2	B	104	THR	43.3
2	B	107	ILE	41.1
2	B	244	THR	40.9
2	B	183	ALA	40.0
2	B	289	ALA	39.6
3	C	96	ASP	39.3
2	B	182	VAL	39.2
2	B	180	GLY	37.1
3	C	113	VAL	34.5
2	B	78	GLN	34.3
2	B	178	LEU	34.2
1	A	14	PHE	34.0
3	C	116	ALA	33.3
3	C	114	LEU	33.3
2	B	103	ARG	33.1
2	B	109	GLU	31.6
2	B	106	LYS	30.8

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Mol	Chain	Res	Type	RSRZ
3	C	258	ASP	30.7
2	B	291	ALA	29.9
2	B	111	GLU	29.5
2	B	285	PRO	28.7
2	B	184	PRO	28.3
2	B	243	VAL	28.0
2	B	151	GLY	27.7
3	C	95	LEU	27.1
3	C	115	LYS	27.0
2	B	77	ILE	26.0
3	C	71	VAL	25.5
1	A	106	GLN	25.3
2	B	245	LYS	23.9
3	C	256	ASN	23.6
2	B	179	THR	23.4
1	A	104	GLN	23.3
1	A	207	VAL	23.2
2	B	242	PRO	22.8
2	B	156	PHE	22.5
1	A	206	VAL	22.4
2	B	203	ILE	22.3
3	C	147	GLY	22.1
3	C	254	ARG	21.7
2	B	73	THR	21.7
3	C	241	MET	21.6
2	B	71	TRP	21.4
3	C	73	ILE	20.4
2	B	300	LEU	20.2
3	C	99	ASN	20.1
3	C	235	VAL	20.0
3	C	206	VAL	19.6
3	C	146	ALA	18.7
2	B	247	MET	18.5
3	C	245	ASN	18.4
2	B	248	ALA	17.6
3	C	117	GLY	17.4
2	B	75	ASP	17.3
2	B	72	LYS	16.9
3	C	94	VAL	16.5
2	B	177	GLN	16.5
3	C	100	SER	16.3
2	B	286	PRO	16.3

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Mol	Chain	Res	Type	RSRZ
2	B	256	VAL	16.2
3	C	184	PHE	16.2
2	B	153	LEU	16.0
1	A	15	PHE	15.9
2	B	301	GLN	15.8
1	A	107	THR	15.4
3	C	243	LEU	15.3
3	C	69	ARG	15.1
2	B	241	ARG	15.0
2	B	288	THR	14.7
2	B	113	ARG	14.5
1	A	164	TYR	14.3
1	A	176	THR	14.2
3	C	133	VAL	14.2
2	B	188	ASN	14.1
2	B	290	SER	14.0
3	C	119	LYS	13.9
2	B	252	VAL	13.3
2	B	185	SER	13.1
2	B	76	ALA	13.0
3	C	204	ASP	12.7
3	C	168	GLN	12.5
3	C	208	GLY	12.5
3	C	236	ASP	12.5
3	C	237	ILE	12.4
1	A	161	ASP	12.3
3	C	120	ALA	12.3
3	C	242	TRP	12.0
1	A	105	SER	12.0
3	C	145	VAL	11.8
3	C	205	LEU	11.8
2	B	114	GLU	11.8
2	B	296	LEU	11.8
2	B	152	ARG	11.7
2	B	154	GLU	11.7
2	B	158	GLU	11.7
3	C	203	TYR	11.6
3	C	59	ASP	11.6
3	C	239	VAL	11.6
2	B	293	VAL	11.4
3	C	112	THR	11.4
2	B	239	CYS	11.4

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Mol	Chain	Res	Type	RSRZ
1	A	13	SER	11.4
2	B	249	PRO	11.3
1	A	19	ASP	11.3
2	B	202	THR	11.2
2	B	157	PHE	11.2
2	B	283	TYR	11.1
3	C	110	PRO	11.0
2	B	250	ASP	11.0
2	B	287	PRO	10.8
3	C	244	SER	10.7
3	C	68	GLN	10.6
3	C	97	GLN	10.6
2	B	251	THR	10.5
2	B	292	ALA	10.5
3	C	72	LEU	10.5
1	A	12	ILE	10.5
3	C	132	ASP	10.3
3	C	118	GLY	9.9
1	A	102	LEU	9.8
1	A	160	SER	9.6
3	C	67	LEU	9.6
3	C	66	PHE	9.5
1	A	205	SER	9.4
2	B	102	ILE	9.2
3	C	185	GLN	9.1
1	A	17	SER	9.1
3	C	78	ILE	9.0
1	A	158	SER	9.0
2	B	163	PRO	9.0
3	C	224	LEU	8.7
2	B	237	PHE	8.7
2	B	189	TYR	8.7
2	B	70	THR	8.7
3	C	98	GLN	8.7
3	C	65	GLN	8.6
2	B	80	PRO	8.5
1	A	163	GLY	8.4
3	C	240	TYR	8.4
3	C	109	LEU	8.3
2	B	181	ALA	8.2
2	B	191	TYR	8.2
3	C	139	LEU	8.2

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Mol	Chain	Res	Type	RSRZ
3	C	93	TYR	8.1
3	C	253	TYR	8.1
3	C	162	THR	8.1
2	B	81	ILE	8.1
3	C	161	ASP	8.0
1	A	103	LYS	8.0
3	C	183	ASP	7.9
3	C	89	PRO	7.9
2	B	74	THR	7.9
3	C	221	THR	7.9
2	B	195	LEU	7.7
3	C	76	ILE	7.6
2	B	11	PRO	7.6
2	B	10	CYS	7.6
2	B	115	THR	7.5
3	C	135	VAL	7.5
2	B	69	LEU	7.5
1	A	172	SER	7.5
3	C	207	THR	7.4
3	C	257	PRO	7.3
1	A	171	PHE	7.3
2	B	190	LYS	7.2
1	A	174	THR	7.2
2	B	146	THR	7.1
2	B	298	VAL	7.0
2	B	257	SER	6.9
2	B	294	GLU	6.9
3	C	255	MET	6.9
3	C	246	ILE	6.9
3	C	141	ALA	6.9
1	A	16	ASP	6.8
3	C	210	GLU	6.8
3	C	111	SER	6.8
2	B	12	LEU	6.7
1	A	173	ASN	6.7
2	B	201	VAL	6.6
3	C	127	LYS	6.6
3	C	251	PRO	6.6
3	C	187	ASP	6.6
2	B	162	ILE	6.5
2	B	149	HIS	6.4
3	C	160	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
3	C	190	VAL	6.4
3	C	134	GLN	6.4
2	B	193	LEU	6.4
2	B	150	THR	6.3
2	B	253	SER	6.3
3	C	70	PRO	6.2
3	C	252	THR	6.2
1	A	177	THR	6.1
2	B	210	ASN	6.1
2	B	1	SER	5.9
3	C	189	SER	5.9
1	A	18	THR	5.9
2	B	144	VAL	5.8
3	C	238	SER	5.8
2	B	9	VAL	5.8
3	C	131	CYS	5.7
1	A	58	ASN	5.7
2	B	192	ILE	5.7
2	B	55	ALA	5.7
3	C	75	ASN	5.7
3	C	61	HIS	5.6
2	B	197	ASN	5.6
2	B	299	GLU	5.6
1	A	175	SER	5.6
3	C	126	PHE	5.6
2	B	145	LYS	5.6
2	B	169	ASN	5.5
2	B	238	LEU	5.5
2	B	155	ILE	5.5
3	C	144	PHE	5.5
2	B	209	SER	5.4
2	B	258	ILE	5.4
2	B	204	ARG	5.4
3	C	101	GLN	5.4
3	C	163	ALA	5.3
2	B	159	PRO	5.3
2	B	223	ASN	5.2
2	B	43	LEU	5.2
2	B	24	LYS	5.2
1	A	108	CYS	5.1
2	B	194	ASP	5.1
1	A	20	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	10	ASN	5.0
3	C	225	GLY	5.0
1	A	53	TRP	5.0
2	B	297	ASN	4.9
1	A	157	ALA	4.8
1	A	198	GLN	4.8
1	A	57	ALA	4.8
2	B	174	ASP	4.8
1	A	162	LYS	4.7
1	A	150	GLN	4.7
2	B	117	VAL	4.7
1	A	170	TYR	4.6
3	C	165	SER	4.6
3	C	128	TYR	4.5
1	A	159	THR	4.5
2	B	56	ILE	4.4
2	B	138	CYS	4.4
2	B	295	VAL	4.4
1	A	11	VAL	4.4
3	C	169	THR	4.4
2	B	205	VAL	4.3
2	B	196	THR	4.3
1	A	204	ARG	4.3
3	C	230	SER	4.3
3	C	192	MET	4.3
2	B	211	LYS	4.3
3	C	83	THR	4.3
2	B	60	CYS	4.3
2	B	208	VAL	4.3
3	C	74	ASP	4.2
1	A	62	PRO	4.2
2	B	160	GLY	4.1
2	B	79	LYS	4.0
2	B	254	ASP	4.0
2	B	132	TYR	4.0
3	C	88	LYS	4.0
3	C	175	THR	3.9
2	B	284	ARG	3.9
2	B	101	SER	3.9
1	A	72	ALA	3.9
1	A	37	VAL	3.9
2	B	272	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	158	ASP	3.9
2	B	118	ILE	3.9
2	B	88	GLY	3.8
3	C	211	ASP	3.8
3	C	60	THR	3.7
3	C	191	GLU	3.7
3	C	232	SER	3.7
3	C	123	LEU	3.7
1	A	121	ALA	3.7
2	B	85	ASP	3.7
1	A	178	GLN	3.7
3	C	222	PRO	3.7
3	C	121	GLN	3.6
2	B	271	GLU	3.6
3	C	182	LEU	3.6
2	B	64	ALA	3.6
1	A	65	ASP	3.5
2	B	236	GLY	3.5
2	B	281	GLN	3.5
3	C	85	ASP	3.5
1	A	61	THR	3.5
2	B	275	LEU	3.5
3	C	159	LYS	3.5
2	B	98	TYR	3.4
2	B	255	ASN	3.3
3	C	226	PRO	3.3
2	B	14	ASN	3.3
3	C	194	ILE	3.3
2	B	16	PRO	3.3
1	A	68	ASN	3.2
3	C	136	LYS	3.2
3	C	142	ASN	3.2
2	B	42	ASP	3.2
1	A	82	SER	3.2
2	B	137	MET	3.2
2	B	276	THR	3.2
2	B	54	MET	3.1
2	B	206	PRO	3.1
3	C	62	SER	3.1
3	C	79	ILE	3.1
3	C	212	PHE	3.1
1	A	109	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	129	LEU	3.0
3	C	202	ALA	3.0
1	A	137	ILE	3.0
2	B	52	ASP	3.0
1	A	22	THR	3.0
3	C	82	THR	3.0
2	B	99	SER	3.0
3	C	209	THR	3.0
3	C	64	ILE	2.9
3	C	122	LYS	2.9
1	A	110	ILE	2.9
3	C	91	SER	2.9
1	A	73	GLN	2.9
1	A	169	MET	2.9
1	A	183	ALA	2.9
2	B	170	ASN	2.9
3	C	229	GLU	2.9
1	A	25	HIS	2.9
2	B	233	SER	2.8
1	A	115	MET	2.8
2	B	235	SER	2.8
2	B	40	LEU	2.8
2	B	93	VAL	2.8
3	C	138	VAL	2.7
2	B	2	LYS	2.7
2	B	123	CYS	2.7
1	A	100	THR	2.7
2	B	282	VAL	2.7
1	A	38	ASN	2.7
3	C	170	SER	2.7
1	A	125	ASN	2.6
2	B	20	TYR	2.6
2	B	46	VAL	2.6
1	A	1	ILE	2.6
3	C	156	TYR	2.6
1	A	197	PRO	2.6
1	A	145	VAL	2.6
2	B	167	THR	2.6
3	C	148	ARG	2.6
1	A	138	ASN	2.6
2	B	274	PRO	2.6
1	A	27	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	174	VAL	2.5
3	C	228	SER	2.5
2	B	131	SER	2.5
2	B	36	PRO	2.5
2	B	13	GLN	2.5
3	C	167	LEU	2.5
2	B	161	VAL	2.5
1	A	63	ILE	2.4
2	B	29	SER	2.4
2	B	133	TRP	2.4
2	B	23	TYR	2.4
2	B	17	ALA	2.4
2	B	30	VAL	2.4
2	B	63	PRO	2.4
1	A	81	LEU	2.4
1	A	60	LYS	2.4
2	B	38	ASN	2.4
1	A	67	THR	2.4
2	B	22	LEU	2.4
1	A	8	ASN	2.4
1	A	156	ILE	2.4
1	A	101	PRO	2.3
1	A	45	THR	2.3
1	A	99	THR	2.3
2	B	121	ALA	2.3
3	C	176	GLY	2.3
1	A	51	ASP	2.3
2	B	218	GLY	2.3
1	A	84	LEU	2.3
2	B	277	SER	2.3
2	B	220	TYR	2.3
2	B	39	GLU	2.3
2	B	219	ILE	2.3
3	C	173	GLY	2.3
3	C	172	ALA	2.3
2	B	216	THR	2.3
2	B	119	ASP	2.3
3	C	223	VAL	2.3
3	C	233	SER	2.2
1	A	203	THR	2.2
1	A	69	THR	2.2
1	A	80	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	143	VAL	2.2
1	A	196	PRO	2.2
2	B	214	LEU	2.2
1	A	189	THR	2.2
1	A	126	VAL	2.2
2	B	37	ASN	2.2
2	B	35	ASP	2.2
2	B	57	GLY	2.2
3	C	150	TYR	2.2
2	B	91	ILE	2.2
1	A	139	PRO	2.2
2	B	97	CYS	2.2
1	A	76	ASP	2.2
3	C	108	THR	2.2
2	B	5	ASN	2.2
2	B	227	ASN	2.2
3	C	195	PRO	2.2
3	C	248	LEU	2.2
3	C	84	ALA	2.2
1	A	59	THR	2.2
1	A	94	TYR	2.2
1	A	194	ILE	2.2
2	B	200	GLU	2.2
1	A	77	TYR	2.1
2	B	139	TYR	2.1
1	A	50	THR	2.1
1	A	83	TYR	2.1
2	B	65	VAL	2.1
3	C	177	TYR	2.1
1	A	78	MET	2.1
1	A	55	LEU	2.1
2	B	59	VAL	2.1
1	A	181	ALA	2.1
2	B	7	GLN	2.1
2	B	142	THR	2.1
2	B	269	VAL	2.1
3	C	63	ILE	2.1
3	C	216	TYR	2.1
2	B	31	PRO	2.1
1	A	41	THR	2.1
1	A	195	GLY	2.0
1	A	188	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	114	LEU	2.0
2	B	270	VAL	2.0
1	A	74	GLY	2.0
1	A	128	GLY	2.0
1	A	47	ARG	2.0
1	A	92	ARG	2.0
1	A	111	ARG	2.0
2	B	32	LEU	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 carbohydrates 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.