Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 11:59 PM JST

PDB ID	:	6IGE
Title	:	Crystal structure of Human Papillomavirus type 33 pentamer
Authors	:	Li, Z.H.; Song, S.; He, M.Z.; Gu, Y.; Li, S.W.
Deposited on	:	2018-09-25
Resolution	:	2.90 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:

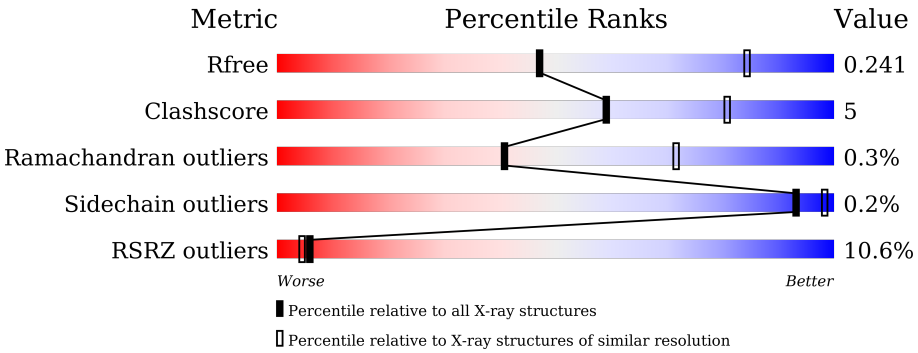
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	A	499	3% 74% 10% 16%
1	B	499	2% 72% 11% 17%
1	C	499	3% 73% 10% 17%
1	D	499	4% 73% 11% 17%
1	E	499	4% 74% 11% 15%
1	F	499	28% 73% 11% 17%

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Mol	Chain	Length	Quality of chain
1	G	499	13% 74% 9% 16%
1	H	499	17% 73% 10% 17%
1	I	499	7% 73% 11% 16%
1	J	499	7% 73% 9% 17%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 33023 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 Major capsid protein L1.

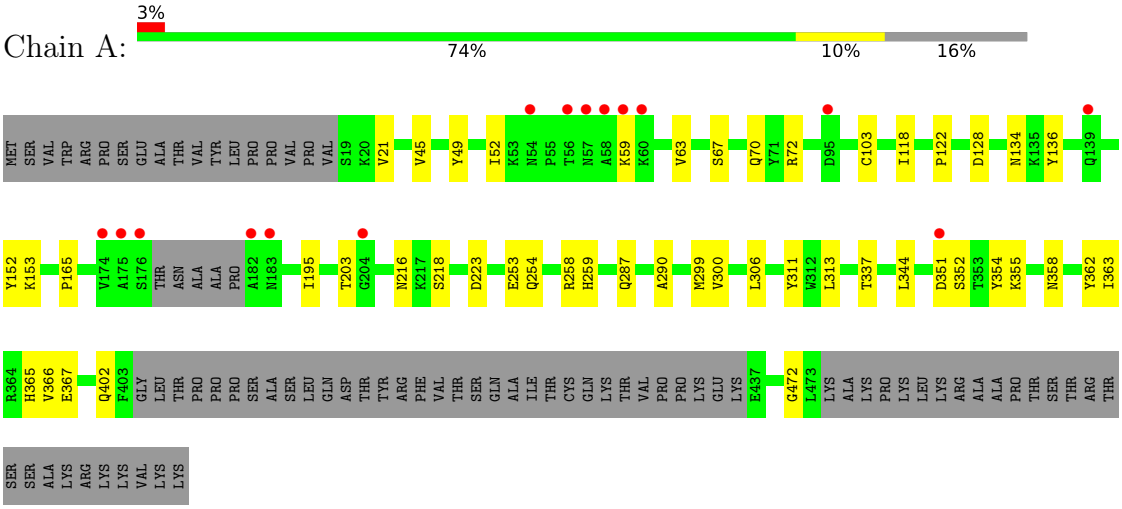
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3309	2113	548	628	20			
1	B	413	Total	C	N	O	S	0	0	0
			3280	2096	542	622	20			
1	C	412	Total	C	N	O	S	0	0	0
			3273	2092	541	620	20			
1	D	416	Total	C	N	O	S	0	0	0
			3300	2108	547	625	20			
1	E	425	Total	C	N	O	S	0	0	0
			3360	2144	557	639	20			
1	F	415	Total	C	N	O	S	0	0	0
			3296	2106	545	625	20			
1	G	417	Total	C	N	O	S	0	0	0
			3310	2115	548	627	20			
1	H	416	Total	C	N	O	S	0	0	0
			3304	2110	547	627	20			
1	I	419	Total	C	N	O	S	0	0	0
			3315	2117	549	629	20			
1	J	412	Total	C	N	O	S	0	0	0
			3276	2095	542	619	20			

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.

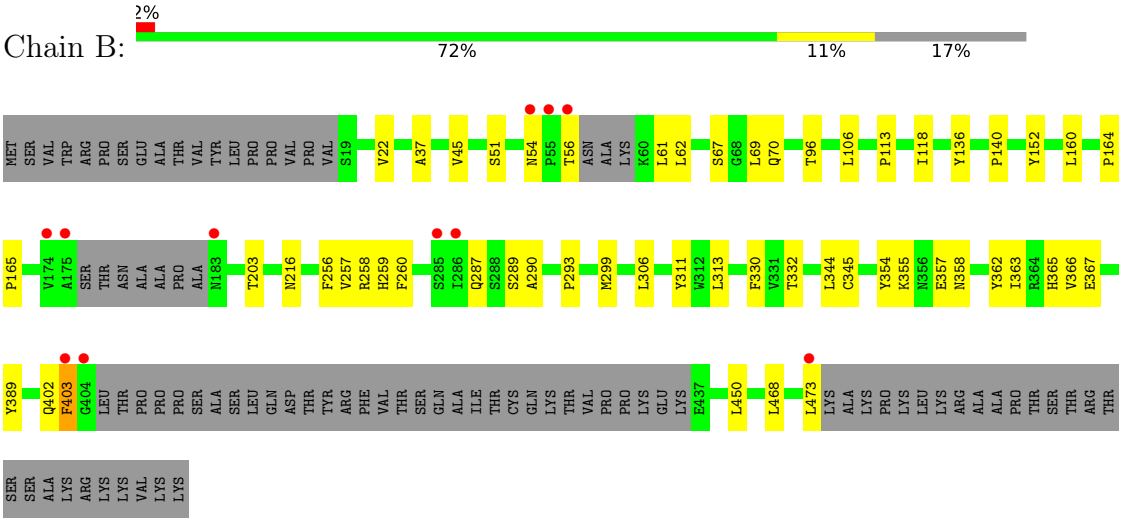
• Molecule 1: Major capsid protein L1

Chain A:



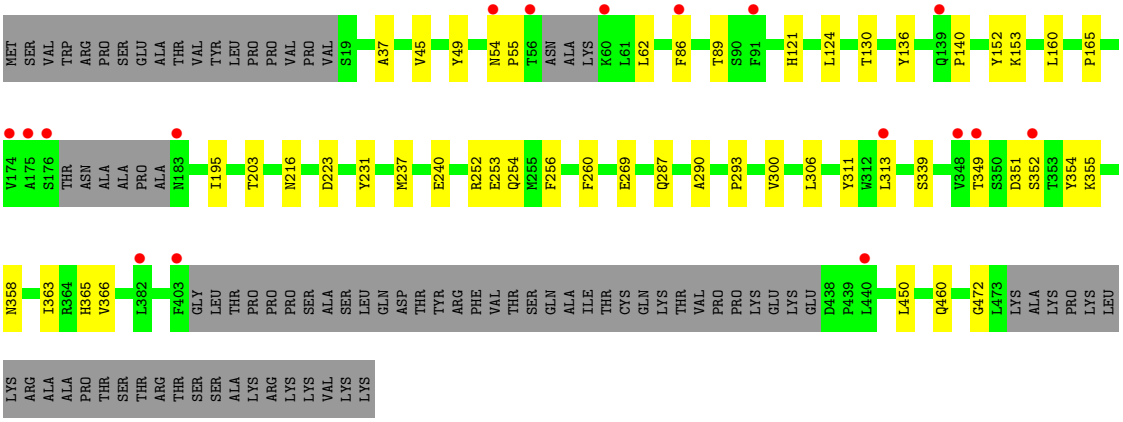
• Molecule 1: Major capsid protein L1

Chain B:



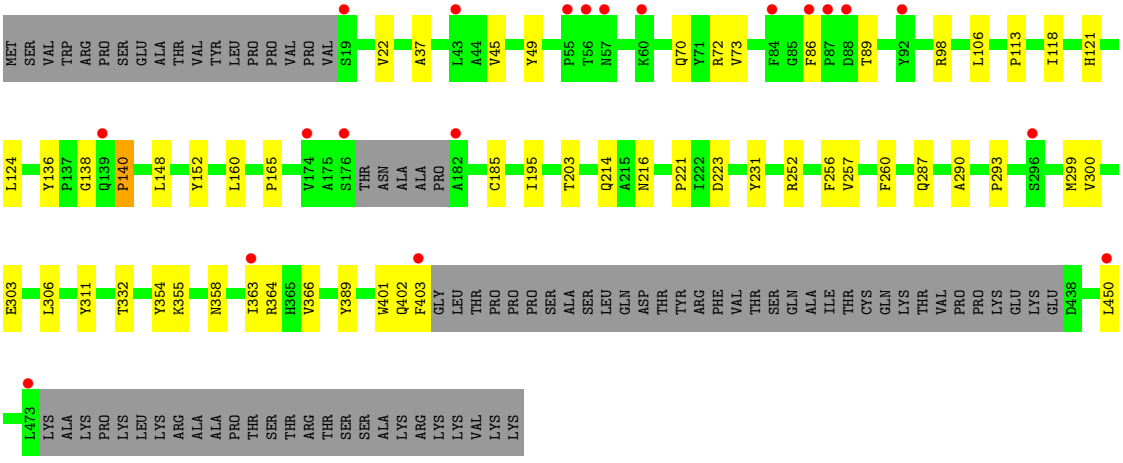
• Molecule 1: Major capsid protein L1

Chain C:



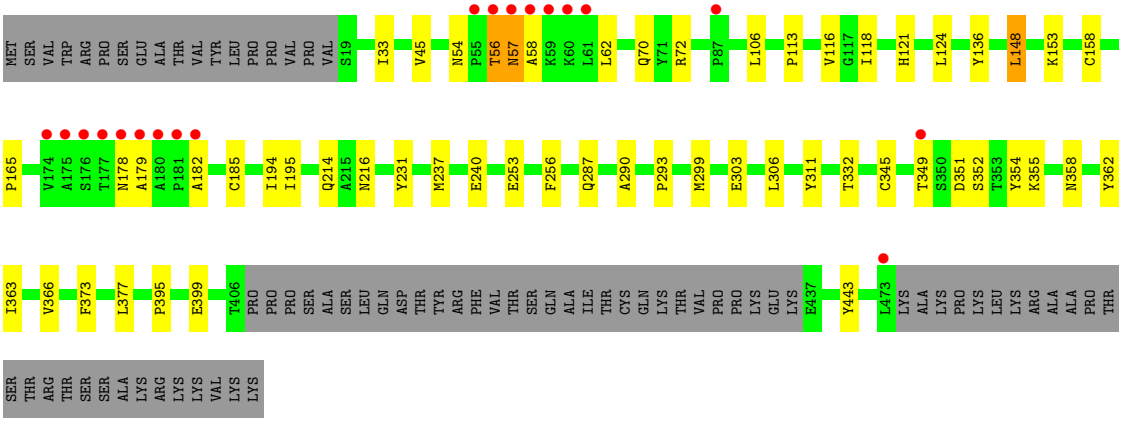
• Molecule 1: Major capsid protein L1

Chain D:

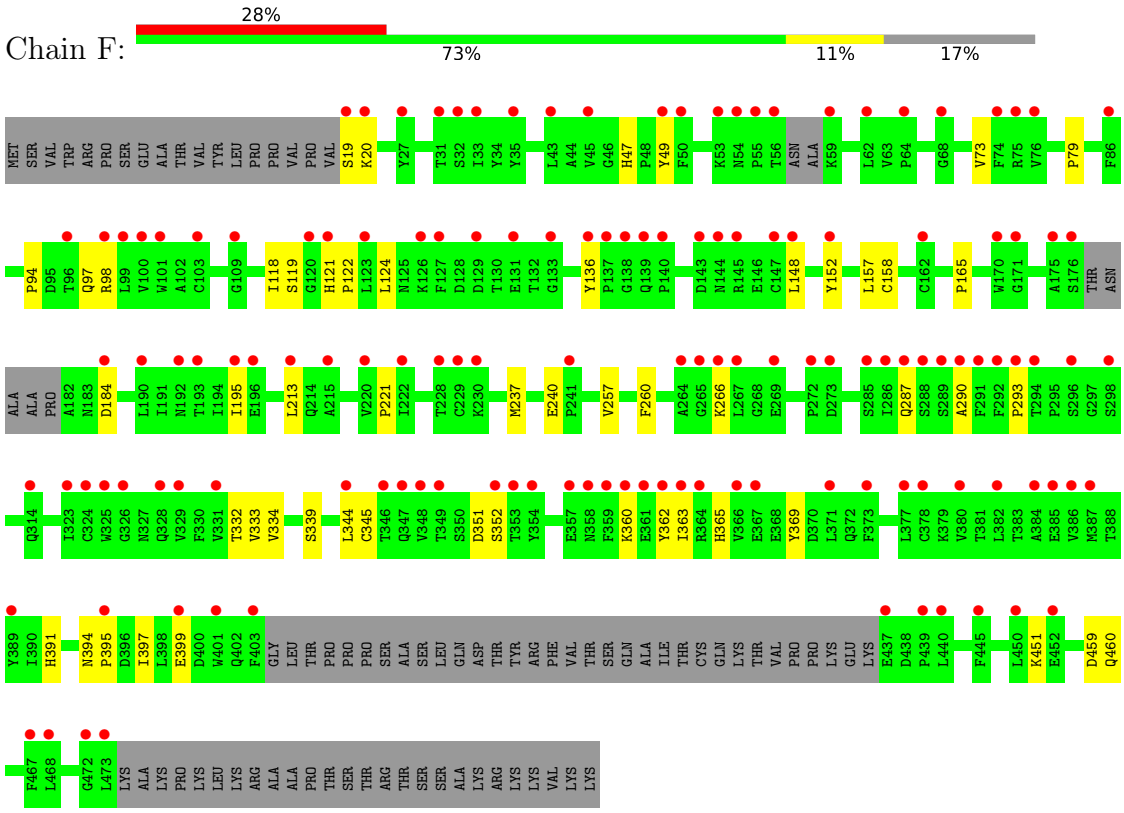


• Molecule 1: Major capsid protein L1

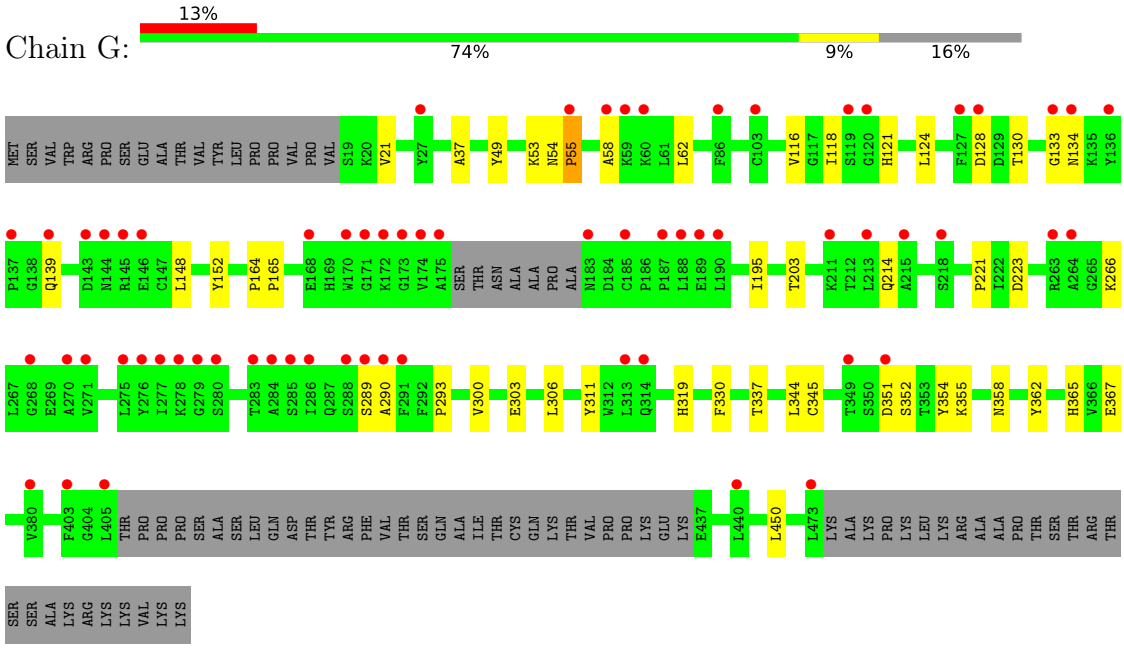
Chain E:



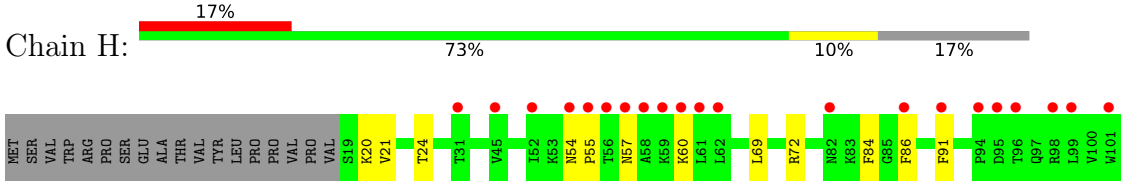
• Molecule 1: Major capsid protein L1

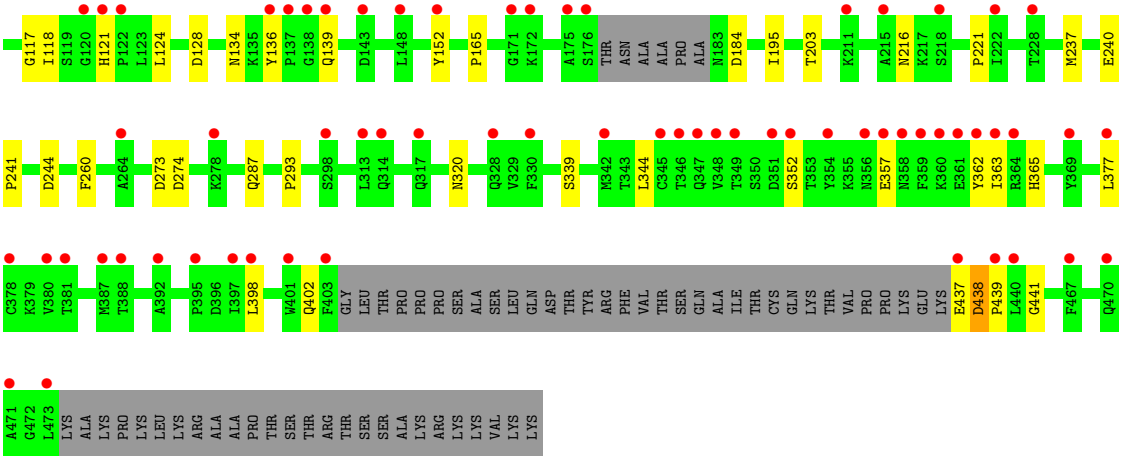


• Molecule 1: Major capsid protein L1



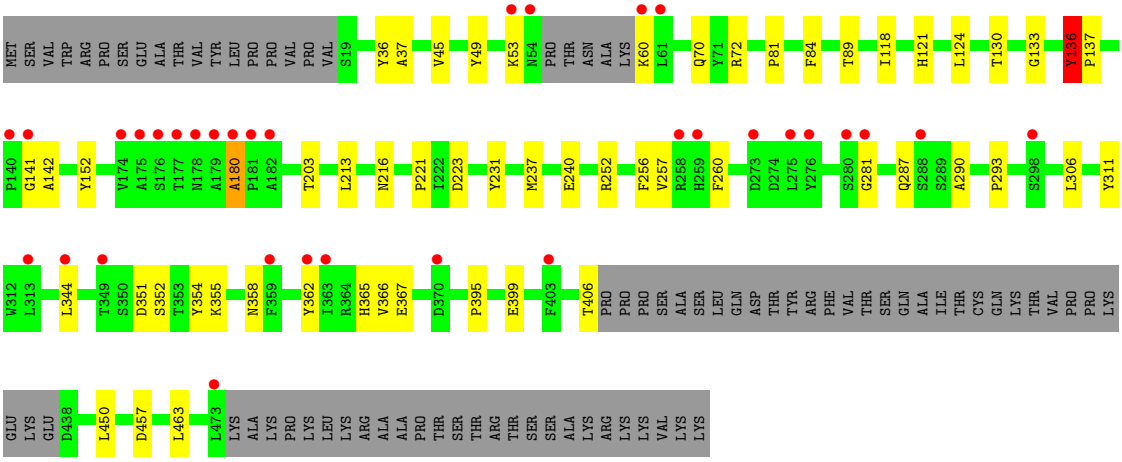
• Molecule 1: Major capsid protein L1





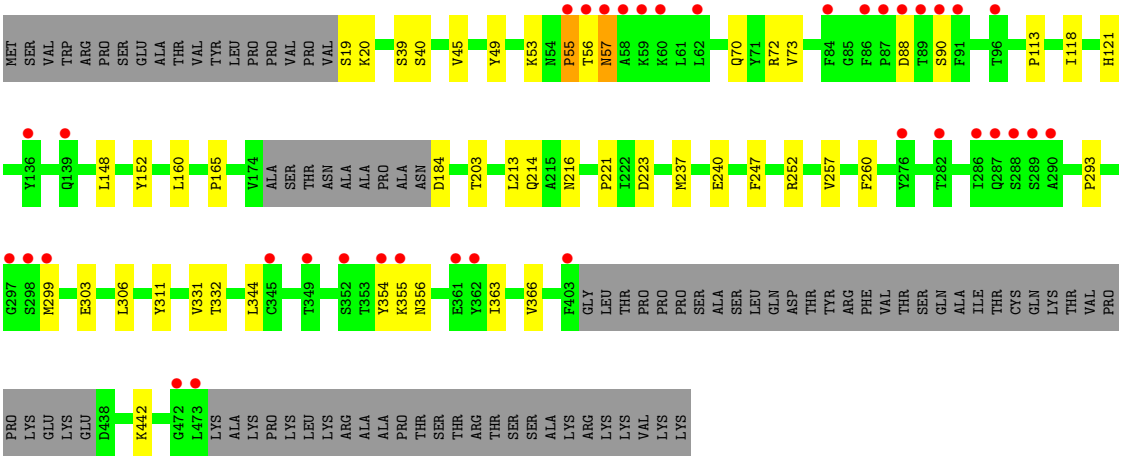
• Molecule 1: Major capsid protein L1

Chain I:



• Molecule 1: Major capsid protein L1

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.83Å 171.94Å 145.69Å 90.00° 97.04° 90.00°	Depositor
Resolution (Å)	48.20 – 2.90 48.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.20-2.90) 98.5 (48.20-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.210 , 0.240 0.210 , 0.241	Depositor DCC
R_{free} test set	5243 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	33023	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.27	0/3395	0.48	0/4604
1	B	0.26	0/3365	0.49	0/4562
1	C	0.26	0/3358	0.47	0/4553
1	D	0.26	0/3386	0.49	0/4592
1	E	0.27	0/3448	0.51	1/4680 (0.0%)
1	F	0.26	0/3381	0.48	0/4583
1	G	0.27	0/3396	0.48	0/4605
1	H	0.26	0/3390	0.47	0/4597
1	I	0.27	0/3401	0.50	0/4614
1	J	0.26	0/3362	0.48	0/4559
All	All	0.26	0/33882	0.48	1/45949 (0.0%)

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	I	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	148	LEU	CA-CB-CG	5.89	128.85	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	136	TYR	Peptide
1	I	180	ALA	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	3309	0	3202	34	0
1	B	3280	0	3170	41	1
1	C	3273	0	3166	38	0
1	D	3300	0	3196	43	0
1	E	3360	0	3254	43	0
1	F	3296	0	3190	42	1
1	G	3310	0	3206	37	0
1	H	3304	0	3197	38	0
1	I	3315	0	3209	41	1
1	J	3276	0	3175	43	1
All	All	33023	0	31965	306	2

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 5.

All (306) 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:I:142:ALA:HB1	1:J:355:LYS:HD2	1.46	0.95
1:J:53:LYS:HG3	1:J:55:PRO:HD3	1.70	0.73
1:J:70:GLN:OE1	1:J:72:ARG:NH2	2.24	0.71
1:F:121:HIS:HB2	1:F:221:PRO:HA	1.74	0.68
1:B:306:LEU:O	1:B:311:TYR:OH	2.07	0.68
1:B:473:LEU:HA	1:H:139:GLN:OE1	1.93	0.68
1:A:118:ILE:HD11	1:B:257:VAL:HG11	1.77	0.67
1:A:70:GLN:OE1	1:A:72:ARG:NH2	2.28	0.67
1:A:122:PRO:HG3	1:B:289:SER:HB3	1.77	0.67
1:G:306:LEU:O	1:G:311:TYR:OH	2.10	0.67
1:G:345:CYS:HB3	1:J:214:GLN:HA	1.78	0.66
1:E:355:LYS:HB2	1:E:358:ASN:OD1	1.97	0.65
1:F:122:PRO:HG3	1:G:289:SER:HB3	1.79	0.63
1:F:290:ALA:HA	1:H:363:ILE:HD11	1.79	0.63
1:H:20:LYS:HZ3	1:I:457:ASP:HB3	1.63	0.63
1:H:57:ASN:HD22	1:H:60:LYS:HE2	1.62	0.63
1:F:47:HIS:HE1	1:F:49:TYR:HB2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:PRO:O	1:F:98:ARG:NH1	2.30	0.63
1:A:306:LEU:O	1:A:311:TYR:OH	2.13	0.62
1:J:306:LEU:O	1:J:311:TYR:OH	2.13	0.62
1:H:184:ASP:OD1	1:I:362:TYR:OH	2.06	0.61
1:F:136:TYR:CZ	1:F:287:GLN:HG3	2.36	0.60
1:F:49:TYR:OH	1:F:118:ILE:O	2.11	0.60
1:C:54:ASN:HB2	1:C:62:LEU:HD11	1.83	0.60
1:D:256:PHE:HB3	1:E:299:MET:HB3	1.84	0.60
1:H:121:HIS:HB3	1:H:124:LEU:HB2	1.85	0.59
1:G:54:ASN:HA	1:G:62:LEU:CD1	2.33	0.58
1:G:121:HIS:HB3	1:G:124:LEU:HB2	1.84	0.58
1:H:20:LYS:NZ	1:I:457:ASP:HB3	2.17	0.58
1:E:306:LEU:O	1:E:311:TYR:OH	2.14	0.58
1:E:349:THR:HB	1:E:358:ASN:ND2	2.18	0.58
1:G:152:TYR:CD1	1:G:203:THR:HB	2.39	0.58
1:I:306:LEU:O	1:I:311:TYR:OH	2.17	0.58
1:C:216:ASN:HB2	1:D:354:TYR:HE2	1.68	0.57
1:A:118:ILE:CD1	1:B:293:PRO:HB3	2.35	0.57
1:F:148:LEU:HD13	1:G:133:GLY:N	2.20	0.57
1:D:70:GLN:OE1	1:D:72:ARG:NH2	2.37	0.57
1:C:306:LEU:O	1:C:311:TYR:OH	2.15	0.57
1:D:136:TYR:CZ	1:D:287:GLN:HG3	2.40	0.57
1:G:303:GLU:OE2	1:J:252:ARG:NE	2.38	0.57
1:I:142:ALA:CB	1:J:355:LYS:HD2	2.28	0.57
1:C:355:LYS:HB2	1:C:358:ASN:OD1	2.04	0.57
1:E:136:TYR:CZ	1:E:287:GLN:HG3	2.40	0.57
1:D:257:VAL:HG11	1:E:118:ILE:HD11	1.86	0.56
1:F:363:ILE:HD11	1:G:290:ALA:HA	1.87	0.56
1:F:119:SER:HB2	1:F:152:TYR:HE2	1.69	0.56
1:H:136:TYR:CZ	1:H:287:GLN:HG3	2.39	0.56
1:I:216:ASN:HB2	1:J:354:TYR:HE2	1.69	0.56
1:B:354:TYR:HE2	1:E:216:ASN:HB2	1.72	0.55
1:H:21:VAL:HG21	1:H:241:PRO:HB2	1.89	0.55
1:F:79:PRO:HD3	1:F:451:LYS:HA	1.87	0.55
1:I:395:PRO:O	1:I:399:GLU:HG3	2.08	0.54
1:F:165:PRO:HG2	1:F:195:ILE:HB	1.89	0.54
1:B:299:MET:HG2	1:E:256:PHE:HB3	1.90	0.54
1:E:70:GLN:OE1	1:E:72:ARG:NH2	2.40	0.54
1:H:54:ASN:OD1	1:H:55:PRO:HD2	2.08	0.54
1:I:290:ALA:HA	1:J:363:ILE:HD11	1.89	0.54
1:D:260:PHE:CD2	1:E:118:ILE:HD13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLY:C	1:G:139:GLN:HE22	2.11	0.53
1:B:136:TYR:CZ	1:B:287:GLN:HG3	2.43	0.53
1:A:290:ALA:HA	1:C:363:ILE:HD11	1.90	0.53
1:D:45:VAL:HG22	1:D:366:VAL:HG12	1.89	0.53
1:D:290:ALA:HA	1:E:363:ILE:HD11	1.91	0.53
1:F:119:SER:HB2	1:F:152:TYR:CE2	2.43	0.53
1:A:216:ASN:HB2	1:C:354:TYR:HE2	1.74	0.53
1:F:184:ASP:OD1	1:H:362:TYR:OH	2.24	0.52
1:H:121:HIS:HB2	1:H:221:PRO:HA	1.89	0.52
1:C:256:PHE:HB3	1:D:299:MET:HG2	1.92	0.52
1:D:306:LEU:O	1:D:311:TYR:OH	2.17	0.51
1:B:468:LEU:O	1:B:473:LEU:N	2.44	0.51
1:F:73:VAL:HG22	1:F:332:THR:HG23	1.92	0.51
1:I:257:VAL:HG11	1:J:118:ILE:HD11	1.92	0.51
1:A:118:ILE:HD13	1:B:260:PHE:CD2	2.46	0.51
1:E:158:CYS:HA	1:E:332:THR:O	2.11	0.51
1:A:344:LEU:HB2	1:A:362:TYR:HB2	1.91	0.51
1:D:136:TYR:CE2	1:D:287:GLN:HG3	2.46	0.51
1:F:157:LEU:HG	1:F:334:VAL:HB	1.92	0.51
1:C:49:TYR:HA	1:C:223:ASP:HB3	1.93	0.51
1:F:47:HIS:CE1	1:F:49:TYR:HB2	2.45	0.51
1:A:152:TYR:CD1	1:A:203:THR:HB	2.45	0.51
1:B:106:LEU:HD22	1:B:160:LEU:HD22	1.93	0.51
1:E:351:ASP:OD1	1:E:352:SER:N	2.43	0.51
1:G:53:LYS:HD2	1:G:58:ALA:HB1	1.92	0.51
1:D:165:PRO:HG2	1:D:195:ILE:HB	1.94	0.50
1:E:45:VAL:HG22	1:E:366:VAL:HG12	1.93	0.50
1:I:256:PHE:HB3	1:J:299:MET:HB3	1.91	0.50
1:J:121:HIS:HB2	1:J:221:PRO:HA	1.93	0.50
1:J:160:LEU:HD13	1:J:247:PHE:HD2	1.76	0.50
1:B:363:ILE:HD11	1:E:290:ALA:HA	1.93	0.50
1:D:252:ARG:NE	1:E:303:GLU:OE2	2.45	0.50
1:D:293:PRO:HB3	1:E:118:ILE:CD1	2.42	0.50
1:J:53:LYS:C	1:J:55:PRO:HD3	2.31	0.50
1:I:37:ALA:HB1	1:I:450:LEU:HD13	1.94	0.50
1:G:351:ASP:OD1	1:G:352:SER:N	2.44	0.50
1:J:53:LYS:HG3	1:J:55:PRO:CD	2.40	0.50
1:C:54:ASN:CB	1:C:62:LEU:HD11	2.41	0.50
1:D:86:PHE:HB2	1:D:89:THR:HG22	1.93	0.50
1:A:299:MET:HB3	1:B:256:PHE:HB3	1.94	0.49
1:F:158:CYS:HA	1:F:332:THR:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:TYR:CE2	1:B:287:GLN:HG3	2.48	0.49
1:E:165:PRO:HG2	1:E:195:ILE:HB	1.93	0.49
1:G:365:HIS:NE2	1:G:367:GLU:OE1	2.41	0.49
1:B:344:LEU:HB2	1:B:362:TYR:HB2	1.95	0.49
1:A:165:PRO:HG2	1:A:195:ILE:HB	1.93	0.49
1:E:121:HIS:HB3	1:E:124:LEU:HB2	1.95	0.49
1:I:70:GLN:OE1	1:I:72:ARG:NH2	2.45	0.49
1:G:118:ILE:HD11	1:J:257:VAL:HG11	1.95	0.49
1:H:128:ASP:OD2	1:H:134:ASN:ND2	2.45	0.49
1:C:130:THR:O	1:D:148:LEU:HD12	2.13	0.49
1:C:237:MET:O	1:C:240:GLU:HG2	2.13	0.49
1:H:273:ASP:OD1	1:H:274:ASP:N	2.45	0.49
1:J:19:SER:OG	1:J:20:LYS:N	2.46	0.49
1:B:37:ALA:HB1	1:B:450:LEU:HD13	1.95	0.48
1:I:142:ALA:O	1:J:355:LYS:HA	2.13	0.48
1:C:62:LEU:N	1:C:62:LEU:HD12	2.29	0.48
1:C:472:GLY:HA3	1:H:352:SER:HB2	1.95	0.48
1:J:56:THR:O	1:J:57:ASN:HB2	2.14	0.48
1:C:121:HIS:HB3	1:C:124:LEU:HB2	1.96	0.48
1:J:45:VAL:HG22	1:J:366:VAL:HG12	1.96	0.48
1:B:45:VAL:HG22	1:B:366:VAL:HG12	1.95	0.48
1:C:37:ALA:HB1	1:C:450:LEU:HD13	1.96	0.48
1:I:130:THR:O	1:J:148:LEU:HD12	2.13	0.48
1:I:237:MET:O	1:I:240:GLU:HG2	2.13	0.48
1:C:349:THR:HB	1:C:358:ASN:ND2	2.29	0.48
1:J:152:TYR:CG	1:J:203:THR:HB	2.49	0.48
1:A:355:LYS:HB2	1:A:358:ASN:ND2	2.29	0.48
1:E:237:MET:O	1:E:240:GLU:HG2	2.14	0.48
1:G:164:PRO:HG3	1:G:330:PHE:CZ	2.49	0.48
1:A:136:TYR:CZ	1:A:287:GLN:HG3	2.48	0.48
1:J:49:TYR:HA	1:J:223:ASP:HB3	1.95	0.48
1:C:136:TYR:CZ	1:C:287:GLN:HG3	2.49	0.47
1:E:178:ASN:HA	1:E:179:ALA:HA	1.54	0.47
1:A:363:ILE:HD11	1:B:290:ALA:HA	1.94	0.47
1:G:124:LEU:HD23	1:G:148:LEU:HD23	1.96	0.47
1:H:260:PHE:CD2	1:I:118:ILE:HD13	2.49	0.47
1:J:237:MET:O	1:J:240:GLU:HG2	2.14	0.47
1:D:401:TRP:O	1:D:402:GLN:HB2	2.15	0.47
1:A:49:TYR:HA	1:A:223:ASP:HB3	1.95	0.47
1:C:45:VAL:HG22	1:C:366:VAL:HG12	1.96	0.47
1:F:339:SER:HA	1:F:365:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:LEU:HD22	1:D:160:LEU:HD22	1.96	0.47
1:F:260:PHE:CD2	1:H:118:ILE:HD13	2.49	0.47
1:G:355:LYS:HB2	1:G:358:ASN:ND2	2.29	0.47
1:G:118:ILE:CD1	1:J:293:PRO:HB3	2.44	0.47
1:I:293:PRO:HB3	1:J:118:ILE:CD1	2.44	0.47
1:C:153:LYS:HE3	1:C:253:GLU:HB3	1.97	0.47
1:D:22:VAL:HG22	1:D:389:TYR:CE2	2.50	0.47
1:G:54:ASN:HA	1:G:62:LEU:HD13	1.95	0.47
1:B:54:ASN:O	1:B:56:THR:N	2.43	0.46
1:F:257:VAL:HG11	1:H:118:ILE:HD11	1.98	0.46
1:B:152:TYR:CG	1:B:203:THR:HB	2.51	0.46
1:C:160:LEU:HD23	1:C:313:LEU:HD11	1.98	0.46
1:E:395:PRO:O	1:E:399:GLU:HG3	2.15	0.46
1:F:351:ASP:OD1	1:F:352:SER:N	2.48	0.46
1:H:69:LEU:HG	1:H:152:TYR:HD2	1.81	0.46
1:B:362:TYR:CE2	1:E:185:CYS:HB2	2.51	0.46
1:F:360:LYS:HA	1:G:266:LYS:HB2	1.98	0.46
1:C:269:GLU:OE1	1:D:364:ARG:NH2	2.38	0.46
1:I:133:GLY:N	1:J:148:LEU:HD13	2.30	0.46
1:I:260:PHE:CD2	1:J:118:ILE:HD13	2.51	0.46
1:A:136:TYR:CE2	1:A:287:GLN:HG3	2.50	0.46
1:A:216:ASN:HD22	1:A:218:SER:HB2	1.81	0.46
1:B:118:ILE:HD11	1:E:293:PRO:HB3	1.98	0.46
1:C:152:TYR:CG	1:C:203:THR:HB	2.51	0.46
1:C:231:TYR:CD1	1:D:113:PRO:HB3	2.51	0.46
1:A:21:VAL:HG22	1:C:460:GLN:OE1	2.15	0.46
1:B:164:PRO:HG3	1:B:330:PHE:CZ	2.51	0.46
1:H:216:ASN:HB2	1:I:354:TYR:HE2	1.81	0.46
1:I:213:LEU:HB3	1:J:344:LEU:HD22	1.97	0.46
1:G:128:ASP:OD2	1:G:134:ASN:ND2	2.48	0.46
1:A:354:TYR:HE2	1:B:216:ASN:HB2	1.80	0.45
1:E:136:TYR:CE2	1:E:287:GLN:HG3	2.52	0.45
1:F:459:ASP:O	1:G:319:HIS:NE2	2.46	0.45
1:A:118:ILE:HD12	1:B:293:PRO:HB3	1.98	0.45
1:G:54:ASN:OD1	1:G:55:PRO:HD2	2.16	0.45
1:B:402:GLN:O	1:B:403:PHE:HD2	1.99	0.45
1:F:460:GLN:OE1	1:G:21:VAL:HG12	2.16	0.45
1:I:136:TYR:CZ	1:I:287:GLN:HG3	2.52	0.45
1:J:88:ASP:OD2	1:J:90:SER:OG	2.22	0.45
1:F:394:ASN:OD1	1:F:397:ILE:HG13	2.17	0.45
1:A:153:LYS:HE3	1:A:253:GLU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASP:OD1	1:A:352:SER:N	2.49	0.45
1:B:113:PRO:HB3	1:E:231:TYR:CD1	2.52	0.45
1:D:355:LYS:HB2	1:D:358:ASN:ND2	2.31	0.45
1:A:52:ILE:HB	1:A:63:VAL:HB	1.98	0.45
1:E:54:ASN:HA	1:E:62:LEU:CD1	2.46	0.45
1:F:237:MET:O	1:F:240:GLU:HG2	2.16	0.45
1:C:54:ASN:OD1	1:C:55:PRO:HD2	2.16	0.45
1:G:121:HIS:HB2	1:G:221:PRO:HA	1.99	0.45
1:A:365:HIS:NE2	1:A:367:GLU:OE2	2.40	0.45
1:B:67:SER:HB3	1:B:70:GLN:HG3	1.98	0.45
1:J:72:ARG:HA	1:J:72:ARG:HD3	1.85	0.45
1:H:344:LEU:HB2	1:H:362:TYR:HB2	1.98	0.45
1:I:45:VAL:HG22	1:I:366:VAL:HG12	1.99	0.45
1:C:293:PRO:HB3	1:D:118:ILE:CD1	2.46	0.44
1:H:165:PRO:HG2	1:H:195:ILE:HB	1.98	0.44
1:I:53:LYS:HG3	1:I:60:LYS:O	2.17	0.44
1:C:165:PRO:HG2	1:C:195:ILE:HB	1.98	0.44
1:D:37:ALA:HB1	1:D:450:LEU:HD13	1.99	0.44
1:G:362:TYR:OH	1:J:184:ASP:HB3	2.17	0.44
1:H:244:ASP:OD1	1:H:320:ASN:ND2	2.31	0.44
1:B:69:LEU:HD22	1:B:203:THR:HG22	1.99	0.44
1:E:54:ASN:C	1:E:56:THR:H	2.21	0.44
1:F:148:LEU:HD12	1:G:130:THR:O	2.17	0.44
1:I:121:HIS:HB3	1:I:124:LEU:HB2	1.99	0.44
1:I:351:ASP:OD1	1:I:352:SER:N	2.50	0.44
1:B:468:LEU:HA	1:B:473:LEU:HB2	1.98	0.44
1:D:231:TYR:CD1	1:E:113:PRO:HB3	2.53	0.44
1:G:37:ALA:HB1	1:G:450:LEU:HD13	1.98	0.44
1:H:72:ARG:HA	1:H:72:ARG:NE	2.33	0.44
1:C:136:TYR:CE2	1:C:287:GLN:HG3	2.53	0.44
1:F:19:SER:OG	1:F:20:LYS:N	2.49	0.44
1:F:345:CYS:HB3	1:G:214:GLN:HA	2.00	0.44
1:G:344:LEU:HD22	1:J:213:LEU:HB3	2.00	0.44
1:B:118:ILE:CD1	1:E:293:PRO:HB3	2.48	0.43
1:C:290:ALA:HA	1:D:363:ILE:HD11	1.99	0.43
1:A:45:VAL:HG22	1:A:366:VAL:HG12	2.01	0.43
1:D:214:GLN:HA	1:E:345:CYS:HB3	1.99	0.43
1:F:344:LEU:HB2	1:F:362:TYR:HB2	1.99	0.43
1:G:354:TYR:HE2	1:J:216:ASN:HB2	1.83	0.43
1:F:266:LYS:HE2	1:H:357:GLU:O	2.19	0.43
1:I:231:TYR:CD1	1:J:113:PRO:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:PRO:HB3	1:D:118:ILE:HD11	2.00	0.43
1:G:116:VAL:HB	1:J:257:VAL:HG23	2.01	0.43
1:H:438:ASP:OD2	1:H:441:GLY:N	2.52	0.43
1:J:39:SER:O	1:J:40:SER:OG	2.31	0.43
1:A:67:SER:HB3	1:A:70:GLN:HG3	2.00	0.43
1:A:128:ASP:OD2	1:A:134:ASN:ND2	2.52	0.43
1:B:160:LEU:HD23	1:B:313:LEU:HD11	2.01	0.43
1:I:81:PRO:HA	1:I:84:PHE:HB2	2.01	0.43
1:F:293:PRO:HB3	1:H:118:ILE:CD1	2.48	0.43
1:J:160:LEU:HD23	1:J:331:VAL:HG22	2.01	0.43
1:D:152:TYR:CG	1:D:203:THR:HB	2.54	0.42
1:E:54:ASN:HA	1:E:62:LEU:HD11	2.01	0.42
1:A:103:CYS:O	1:A:313:LEU:HD12	2.19	0.42
1:A:254:GLN:HA	1:C:300:VAL:O	2.18	0.42
1:D:121:HIS:HB2	1:D:221:PRO:HA	2.01	0.42
1:H:24:THR:HG23	1:H:320:ASN:HA	2.01	0.42
1:B:258:ARG:HG3	1:B:259:HIS:CD2	2.55	0.42
1:F:136:TYR:CE2	1:F:287:GLN:HG3	2.54	0.42
1:G:165:PRO:HG2	1:G:195:ILE:HB	2.00	0.42
1:D:121:HIS:HB3	1:D:124:LEU:HB2	2.01	0.42
1:D:216:ASN:HB2	1:E:354:TYR:HE2	1.84	0.42
1:G:118:ILE:HD13	1:J:260:PHE:CD2	2.54	0.42
1:H:84:PHE:HB3	1:H:86:PHE:CE2	2.55	0.42
1:I:121:HIS:HB2	1:I:221:PRO:HA	2.00	0.42
1:I:142:ALA:O	1:J:356:ASN:N	2.45	0.42
1:I:152:TYR:CG	1:I:203:THR:HB	2.55	0.42
1:I:344:LEU:HB2	1:I:362:TYR:HB2	2.01	0.42
1:I:365:HIS:NE2	1:I:367:GLU:OE2	2.43	0.42
1:B:345:CYS:HB3	1:E:214:GLN:HA	2.00	0.42
1:C:252:ARG:NE	1:D:303:GLU:OE2	2.53	0.42
1:F:391:HIS:CD2	1:F:395:PRO:HA	2.54	0.42
1:I:72:ARG:HA	1:I:72:ARG:HD3	1.91	0.42
1:B:51:SER:HB2	1:B:61:LEU:HD22	2.02	0.42
1:D:98:ARG:HA	1:D:98:ARG:HD3	1.78	0.42
1:F:213:LEU:HB3	1:H:344:LEU:HD22	2.01	0.42
1:A:300:VAL:HG11	1:A:337:THR:HA	2.02	0.42
1:B:165:PRO:HG3	1:B:332:THR:OG1	2.20	0.42
1:D:49:TYR:HA	1:D:223:ASP:HB3	2.02	0.42
1:J:73:VAL:HG22	1:J:332:THR:HG23	2.00	0.42
1:F:121:HIS:HB3	1:F:124:LEU:HB2	2.02	0.42
1:G:49:TYR:HA	1:G:223:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:TYR:CG	1:H:203:THR:HB	2.54	0.42
1:H:339:SER:HA	1:H:365:HIS:CE1	2.54	0.42
1:F:118:ILE:CD1	1:G:293:PRO:HB3	2.50	0.42
1:I:355:LYS:HB2	1:I:358:ASN:ND2	2.34	0.42
1:B:355:LYS:HB2	1:B:358:ASN:ND2	2.35	0.41
1:E:106:LEU:HD13	1:E:373:PHE:CE2	2.55	0.41
1:I:36:TYR:HE1	1:I:463:LEU:HB3	1.85	0.41
1:B:62:LEU:HD21	1:E:182:ALA:HB1	2.03	0.41
1:H:117:GLY:HA3	1:H:339:SER:O	2.20	0.41
1:C:260:PHE:CD2	1:D:118:ILE:HD13	2.56	0.41
1:E:57:ASN:HA	1:E:58:ALA:HA	1.82	0.41
1:A:59:LYS:H	1:A:59:LYS:HD2	1.84	0.41
1:C:339:SER:HA	1:C:365:HIS:CE1	2.56	0.41
1:C:351:ASP:OD1	1:C:352:SER:N	2.53	0.41
1:I:49:TYR:HA	1:I:223:ASP:HB3	2.02	0.41
1:E:33:ILE:HB	1:E:377:LEU:HB3	2.03	0.41
1:F:97:GLN:O	1:F:98:ARG:NH1	2.46	0.41
1:H:91:PHE:CZ	1:H:377:LEU:HD21	2.56	0.41
1:H:437:GLU:O	1:H:439:PRO:HD3	2.21	0.41
1:J:165:PRO:HG3	1:J:332:THR:OG1	2.20	0.41
1:B:96:THR:HG21	1:I:281:GLY:O	2.21	0.41
1:B:365:HIS:NE2	1:B:367:GLU:OE1	2.44	0.41
1:D:138:GLY:O	1:D:140:PRO:HD3	2.21	0.41
1:D:185:CYS:HB2	1:E:362:TYR:CD2	2.56	0.41
1:A:258:ARG:HG3	1:A:259:HIS:CD2	2.56	0.41
1:C:254:GLN:HA	1:D:300:VAL:O	2.21	0.41
1:E:194:ILE:HD12	1:E:443:TYR:CE2	2.55	0.41
1:D:402:GLN:C	1:D:403:PHE:CD1	2.95	0.40
1:E:153:LYS:HE3	1:E:253:GLU:HB3	2.01	0.40
1:C:86:PHE:HB2	1:C:89:THR:HG22	2.03	0.40
1:F:391:HIS:NE2	1:F:395:PRO:HB3	2.36	0.40
1:G:300:VAL:HG11	1:G:337:THR:HA	2.03	0.40
1:H:136:TYR:CE2	1:H:287:GLN:HG3	2.57	0.40
1:H:237:MET:O	1:H:240:GLU:HG2	2.22	0.40
1:H:293:PRO:HB3	1:I:118:ILE:CD1	2.51	0.40
1:B:22:VAL:HG22	1:B:389:TYR:CE2	2.56	0.40
1:D:257:VAL:HG23	1:E:116:VAL:HB	2.03	0.40
1:F:333:VAL:HG11	1:F:369:TYR:HE2	1.86	0.40
1:F:339:SER:HA	1:F:365:HIS:HE1	1.86	0.40
1:I:252:ARG:NE	1:J:303:GLU:OE2	2.55	0.40
1:C:260:PHE:HD2	1:D:118:ILE:HD13	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:VAL:HG22	1:D:332:THR:HG23	2.03	0.40
1:E:72:ARG:HD3	1:E:72:ARG:HA	1.83	0.40

All (2) 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:B:357:GLU:OE1	1:I:89:THR:OG1[1_554]	2.14	0.06
1:F:399:GLU:OE2	1:J:442:LYS:NZ[2_546]	2.16	0.04

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	411/499 (82%)	395 (96%)	15 (4%)	1 (0%)	47	78
1	B	405/499 (81%)	392 (97%)	12 (3%)	1 (0%)	47	78
1	C	404/499 (81%)	392 (97%)	11 (3%)	1 (0%)	47	78
1	D	410/499 (82%)	399 (97%)	10 (2%)	1 (0%)	47	78
1	E	421/499 (84%)	404 (96%)	17 (4%)	0	100	100
1	F	407/499 (82%)	394 (97%)	13 (3%)	0	100	100
1	G	411/499 (82%)	395 (96%)	15 (4%)	1 (0%)	47	78
1	H	410/499 (82%)	396 (97%)	12 (3%)	2 (0%)	29	61
1	I	413/499 (83%)	392 (95%)	17 (4%)	4 (1%)	15	45
1	J	406/499 (81%)	390 (96%)	14 (3%)	2 (0%)	29	61
All	All	4098/4990 (82%)	3949 (96%)	136 (3%)	13 (0%)	41	71

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	136	TYR
1	I	137	PRO
1	I	180	ALA
1	J	57	ASN
1	I	141	GLY
1	H	402	GLN
1	H	438	ASP
1	A	402	GLN
1	G	55	PRO
1	B	140	PRO
1	C	140	PRO
1	D	140	PRO
1	J	55	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	367/439 (84%)	367 (100%)	0	100	100
1	B	364/439 (83%)	363 (100%)	1 (0%)	92	98
1	C	364/439 (83%)	364 (100%)	0	100	100
1	D	366/439 (83%)	366 (100%)	0	100	100
1	E	372/439 (85%)	369 (99%)	3 (1%)	81	94
1	F	366/439 (83%)	366 (100%)	0	100	100
1	G	367/439 (84%)	367 (100%)	0	100	100
1	H	367/439 (84%)	366 (100%)	1 (0%)	92	98
1	I	367/439 (84%)	365 (100%)	2 (0%)	88	96
1	J	364/439 (83%)	364 (100%)	0	100	100
All	All	3664/4390 (84%)	3657 (100%)	7 (0%)	93	98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	403	PHE

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Mol	Chain	Res	Type
1	E	56	THR
1	E	57	ASN
1	E	148	LEU
1	H	398	LEU
1	I	136	TYR
1	I	406	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	347	GLN
1	I	178	ASN

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, 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	417/499 (83%)	0.26	15 (3%) 42 37	35, 59, 101, 151	0
1	B	413/499 (82%)	0.13	11 (2%) 54 50	31, 49, 88, 121	0
1	C	412/499 (82%)	0.40	17 (4%) 37 32	43, 68, 99, 164	0
1	D	416/499 (83%)	0.33	20 (4%) 30 27	39, 61, 105, 140	0
1	E	425/499 (85%)	0.26	19 (4%) 33 29	31, 47, 95, 178	0
1	F	415/499 (83%)	1.64	138 (33%) 0 0	64, 116, 147, 183	0
1	G	417/499 (83%)	0.91	65 (15%) 2 1	48, 82, 139, 163	0
1	H	416/499 (83%)	1.24	86 (20%) 1 0	64, 97, 141, 170	0
1	I	419/499 (83%)	0.54	33 (7%) 12 10	38, 65, 115, 182	0
1	J	412/499 (82%)	0.59	37 (8%) 9 7	42, 71, 120, 149	0
All	All	4162/4990 (83%)	0.63	441 (10%) 6 4	31, 70, 133, 183	0

All (441) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	179	ALA	14.0
1	I	178	ASN	9.6
1	F	473	LEU	9.5
1	F	176	SER	9.2
1	E	181	PRO	9.1
1	E	178	ASN	8.8
1	B	175	ALA	8.7
1	H	58	ALA	7.9
1	H	354	TYR	7.9
1	E	180	ALA	7.9
1	I	180	ALA	7.8
1	G	183	ASN	7.7
1	H	54	ASN	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	59	LYS	7.5
1	I	181	PRO	7.1
1	H	364	ARG	6.9
1	F	378	CYS	6.8
1	G	144	ASN	6.8
1	H	55	PRO	6.6
1	D	57	ASN	6.5
1	I	179	ALA	6.2
1	B	56	THR	6.1
1	F	54	ASN	6.1
1	H	61	LEU	5.8
1	F	56	THR	5.8
1	G	405	LEU	5.8
1	I	176	SER	5.7
1	F	286	ILE	5.6
1	A	58	ALA	5.6
1	E	57	ASN	5.6
1	G	173	GLY	5.5
1	G	440	LEU	5.5
1	G	277	ILE	5.5
1	D	473	LEU	5.4
1	D	55	PRO	5.4
1	H	403	PHE	5.3
1	J	473	LEU	5.3
1	E	58	ALA	5.3
1	C	176	SER	5.3
1	H	349	THR	5.2
1	H	361	GLU	5.2
1	F	133	GLY	5.1
1	F	354	TYR	5.1
1	H	358	ASN	5.0
1	F	292	PHE	5.0
1	A	182	ALA	5.0
1	D	19	SER	4.9
1	B	174	VAL	4.9
1	C	56	THR	4.8
1	F	171	GLY	4.8
1	H	91	PHE	4.8
1	F	269	GLU	4.8
1	H	176	SER	4.8
1	F	59	LYS	4.8
1	F	361	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	H	348	VAL	4.8
1	F	99	LEU	4.8
1	F	285	SER	4.7
1	C	175	ALA	4.7
1	F	349	THR	4.7
1	E	176	SER	4.6
1	I	473	LEU	4.6
1	G	289	SER	4.6
1	I	281	GLY	4.5
1	F	389	TYR	4.5
1	F	403	PHE	4.5
1	J	62	LEU	4.5
1	F	385	GLU	4.4
1	F	364	ARG	4.4
1	F	362	TYR	4.4
1	G	264	ALA	4.4
1	H	387	MET	4.4
1	H	101	TRP	4.4
1	F	175	ALA	4.3
1	J	282	THR	4.3
1	F	265	GLY	4.3
1	F	143	ASP	4.3
1	H	356	ASN	4.2
1	D	87	PRO	4.2
1	H	360	LYS	4.2
1	H	359	PHE	4.2
1	E	175	ALA	4.2
1	J	91	PHE	4.2
1	J	355	LYS	4.2
1	E	177	THR	4.2
1	G	351	ASP	4.1
1	H	57	ASN	4.1
1	F	267	LEU	4.1
1	F	440	LEU	4.1
1	H	175	ALA	4.0
1	H	357	GLU	4.0
1	H	59	LYS	4.0
1	J	59	LYS	4.0
1	F	49	TYR	4.0
1	F	353	THR	4.0
1	F	348	VAL	4.0
1	G	119	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	139	GLN	4.0
1	G	145	ARG	4.0
1	F	140	PRO	4.0
1	A	176	SER	4.0
1	G	137	PRO	3.9
1	I	177	THR	3.9
1	F	399	GLU	3.9
1	J	88	ASP	3.9
1	F	264	ALA	3.9
1	G	175	ALA	3.9
1	G	280	SER	3.9
1	G	283	THR	3.8
1	B	473	LEU	3.8
1	D	176	SER	3.8
1	G	276	TYR	3.8
1	G	275	LEU	3.8
1	I	403	PHE	3.8
1	E	174	VAL	3.8
1	G	146	GLU	3.7
1	F	230	LYS	3.7
1	F	357	GLU	3.7
1	G	284	ALA	3.7
1	E	59	LYS	3.7
1	J	60	LYS	3.7
1	J	56	THR	3.7
1	F	273	ASP	3.7
1	J	58	ALA	3.7
1	G	188	LEU	3.7
1	G	174	VAL	3.6
1	D	56	THR	3.6
1	F	359	PHE	3.6
1	F	45	VAL	3.6
1	H	122	PRO	3.6
1	G	285	SER	3.6
1	G	185	CYS	3.6
1	H	363	ILE	3.6
1	B	403	PHE	3.5
1	G	171	GLY	3.5
1	F	445	PHE	3.5
1	B	404	GLY	3.5
1	G	127	PHE	3.5
1	G	170	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	440	LEU	3.5
1	G	286	ILE	3.5
1	G	290	ALA	3.5
1	J	354	TYR	3.5
1	F	190	LEU	3.4
1	F	43	LEU	3.4
1	F	100	VAL	3.4
1	I	313	LEU	3.4
1	F	228	THR	3.3
1	F	329	VAL	3.3
1	G	291	PHE	3.3
1	G	58	ALA	3.3
1	G	268	GLY	3.3
1	F	53	LYS	3.3
1	F	64	PRO	3.3
1	F	241	PRO	3.3
1	D	182	ALA	3.3
1	J	89	THR	3.3
1	F	298	SER	3.3
1	G	473	LEU	3.3
1	G	279	GLY	3.3
1	F	468	LEU	3.3
1	F	74	PHE	3.2
1	C	60	LYS	3.2
1	A	57	ASN	3.2
1	B	55	PRO	3.2
1	F	437	GLU	3.2
1	H	98	ARG	3.2
1	F	293	PRO	3.2
1	F	352	SER	3.2
1	H	362	TYR	3.2
1	H	94	PRO	3.2
1	F	120	GLY	3.2
1	A	60	LYS	3.2
1	B	285	SER	3.2
1	G	143	ASP	3.2
1	J	139	GLN	3.2
1	F	439	PRO	3.2
1	G	134	ASN	3.1
1	F	147	CYS	3.1
1	C	86	PHE	3.1
1	I	362	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	98	ARG	3.1
1	F	145	ARG	3.1
1	F	380	VAL	3.1
1	F	386	VAL	3.1
1	H	437	GLU	3.1
1	H	351	ASP	3.1
1	F	31	THR	3.1
1	E	349	THR	3.0
1	D	86	PHE	3.0
1	I	344	LEU	3.0
1	A	56	THR	3.0
1	F	86	PHE	3.0
1	F	123	LEU	3.0
1	H	56	THR	3.0
1	J	90	SER	3.0
1	A	95	ASP	3.0
1	F	55	PRO	2.9
1	G	133	GLY	2.9
1	D	450	LEU	2.9
1	F	127	PHE	2.9
1	A	175	ALA	2.9
1	J	55	PRO	2.9
1	H	60	LYS	2.9
1	E	60	LYS	2.9
1	E	61	LEU	2.9
1	H	314	GLN	2.9
1	H	346	THR	2.9
1	I	60	LYS	2.9
1	F	162	CYS	2.9
1	F	325	TRP	2.9
1	F	347	GLN	2.9
1	F	192	ASN	2.8
1	G	288	SER	2.8
1	J	289	SER	2.8
1	I	175	ALA	2.8
1	J	286	ILE	2.8
1	H	401	TRP	2.8
1	I	280	SER	2.8
1	I	141	GLY	2.8
1	A	174	VAL	2.8
1	G	270	ALA	2.8
1	J	86	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	170	TRP	2.8
1	F	358	ASN	2.8
1	H	328	GLN	2.8
1	H	352	SER	2.8
1	A	351	ASP	2.8
1	F	346	THR	2.8
1	F	287	GLN	2.8
1	F	33	ILE	2.8
1	F	129	ASP	2.8
1	E	55	PRO	2.7
1	F	377	LEU	2.7
1	D	88	ASP	2.7
1	F	148	LEU	2.7
1	F	289	SER	2.7
1	J	288	SER	2.7
1	F	384	ALA	2.7
1	F	68	GLY	2.7
1	I	288	SER	2.7
1	H	139	GLN	2.7
1	H	347	GLN	2.7
1	F	101	TRP	2.7
1	I	259	HIS	2.7
1	B	54	ASN	2.6
1	F	137	PRO	2.6
1	F	395	PRO	2.6
1	I	182	ALA	2.6
1	F	472	GLY	2.6
1	J	403	PHE	2.6
1	F	323	ILE	2.6
1	F	121	HIS	2.6
1	C	440	LEU	2.6
1	F	19	SER	2.6
1	I	359	PHE	2.6
1	H	218	SER	2.6
1	G	172	LYS	2.6
1	J	472	GLY	2.6
1	G	215	ALA	2.6
1	J	84	PHE	2.6
1	D	43	LEU	2.6
1	F	152	TYR	2.6
1	J	352	SER	2.6
1	F	131	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	403	PHE	2.6
1	F	75	ARG	2.6
1	C	382	LEU	2.6
1	F	373	PHE	2.6
1	F	109	GLY	2.5
1	G	349	THR	2.5
1	H	120	GLY	2.5
1	H	345	CYS	2.5
1	I	298	SER	2.5
1	F	314	GLN	2.5
1	E	182	ALA	2.5
1	F	367	GLU	2.5
1	F	222	ILE	2.5
1	F	288	SER	2.5
1	F	96	THR	2.5
1	H	330	PHE	2.5
1	B	183	ASN	2.5
1	H	148	LEU	2.5
1	F	76	VAL	2.5
1	G	86	PHE	2.5
1	J	136	TYR	2.5
1	J	349	THR	2.5
1	H	317	GLN	2.5
1	J	96	THR	2.5
1	F	363	ILE	2.5
1	F	382	LEU	2.5
1	I	363	ILE	2.5
1	I	140	PRO	2.4
1	F	50	PHE	2.4
1	H	99	LEU	2.4
1	I	174	VAL	2.4
1	H	215	ALA	2.4
1	F	126	LYS	2.4
1	G	55	PRO	2.4
1	C	174	VAL	2.4
1	G	120	GLY	2.4
1	F	136	TYR	2.4
1	H	96	THR	2.4
1	D	139	GLN	2.4
1	G	314	GLN	2.4
1	G	278	LYS	2.4
1	G	218	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	54	ASN	2.4
1	H	471	ALA	2.4
1	C	403	PHE	2.4
1	D	92	TYR	2.4
1	H	228	THR	2.4
1	H	278	LYS	2.4
1	I	53	LYS	2.4
1	F	215	ALA	2.4
1	H	264	ALA	2.4
1	B	286	ILE	2.4
1	D	363	ILE	2.4
1	E	56	THR	2.4
1	C	54	ASN	2.4
1	H	473	LEU	2.4
1	H	172	LYS	2.4
1	H	439	PRO	2.4
1	F	184	ASP	2.4
1	G	263	ARG	2.4
1	H	138	GLY	2.3
1	J	290	ALA	2.3
1	G	213	LEU	2.3
1	G	313	LEU	2.3
1	D	403	PHE	2.3
1	F	291	PHE	2.3
1	F	196	GLU	2.3
1	F	62	LEU	2.3
1	H	380	VAL	2.3
1	F	296	SER	2.3
1	F	328	GLN	2.3
1	G	190	LEU	2.3
1	H	398	LEU	2.3
1	I	275	LEU	2.3
1	H	470	GLN	2.3
1	C	313	LEU	2.3
1	F	229	CYS	2.3
1	H	342	MET	2.3
1	I	61	LEU	2.3
1	J	345	CYS	2.3
1	F	467	PHE	2.3
1	C	352	SER	2.3
1	G	380	VAL	2.3
1	F	401	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	369	TYR	2.3
1	J	276	TYR	2.3
1	G	103	CYS	2.3
1	F	331	VAL	2.3
1	H	82	ASN	2.3
1	G	187	PRO	2.3
1	J	362	TYR	2.3
1	D	84	PHE	2.3
1	D	174	VAL	2.2
1	F	366	VAL	2.2
1	I	349	THR	2.2
1	F	20	LYS	2.2
1	H	313	LEU	2.2
1	F	27	TYR	2.2
1	H	121	HIS	2.2
1	F	452	GLU	2.2
1	G	128	ASP	2.2
1	H	388	THR	2.2
1	F	344	LEU	2.2
1	I	258	ARG	2.2
1	F	360	LYS	2.2
1	F	213	LEU	2.2
1	H	171	GLY	2.2
1	H	378	CYS	2.2
1	J	287	GLN	2.2
1	F	35	TYR	2.2
1	G	189	GLU	2.2
1	J	297	GLY	2.2
1	A	183	ASN	2.2
1	H	211	LYS	2.2
1	F	195	ILE	2.2
1	G	136	TYR	2.2
1	H	45	VAL	2.2
1	F	387	MET	2.2
1	H	137	PRO	2.1
1	H	136	TYR	2.1
1	E	473	LEU	2.1
1	G	59	LYS	2.1
1	D	296	SER	2.1
1	F	103	CYS	2.1
1	G	211	LYS	2.1
1	H	397	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	361	GLU	2.1
1	H	298	SER	2.1
1	C	349	THR	2.1
1	H	143	ASP	2.1
1	C	183	ASN	2.1
1	F	144	ASN	2.1
1	C	348	VAL	2.1
1	D	60	LYS	2.1
1	J	298	SER	2.1
1	H	31	THR	2.1
1	F	371	LEU	2.1
1	H	95	ASP	2.1
1	A	54	ASN	2.1
1	F	220	VAL	2.1
1	H	222	ILE	2.1
1	G	271	VAL	2.1
1	G	60	LYS	2.1
1	F	272	PRO	2.1
1	G	168	GLU	2.1
1	F	266	LYS	2.1
1	F	324	CYS	2.1
1	H	52	ILE	2.1
1	I	273	ASP	2.1
1	A	204	GLY	2.1
1	H	395	PRO	2.1
1	C	139	GLN	2.0
1	F	290	ALA	2.0
1	H	152	TYR	2.0
1	H	392	ALA	2.0
1	I	276	TYR	2.0
1	F	326	GLY	2.0
1	J	87	PRO	2.0
1	F	138	GLY	2.0
1	G	27	TYR	2.0
1	C	91	PHE	2.0
1	E	87	PRO	2.0
1	F	450	LEU	2.0
1	H	86	PHE	2.0
1	H	467	PHE	2.0
1	F	32	SER	2.0
1	F	294	THR	2.0
1	H	62	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	377	LEU	2.0
1	I	370	ASP	2.0
1	F	193	THR	2.0
1	H	381	THR	2.0
1	J	299	MET	2.0
1	A	139	GLN	2.0
1	G	139	GLN	2.0
1	J	57	ASN	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 monosaccharides 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.