



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2022 – 06:27 PM JST

PDB ID : 7F8I  
Title : Crystal structure of HPV6 L1 pentamer  
Authors : Wang, Z.P.; Wang, D.N.; Gu, Y.; Li, S.W.  
Deposited on : 2021-07-02  
Resolution : 3.37 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](mailto: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>.

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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	:	2.29
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)	:	2.29



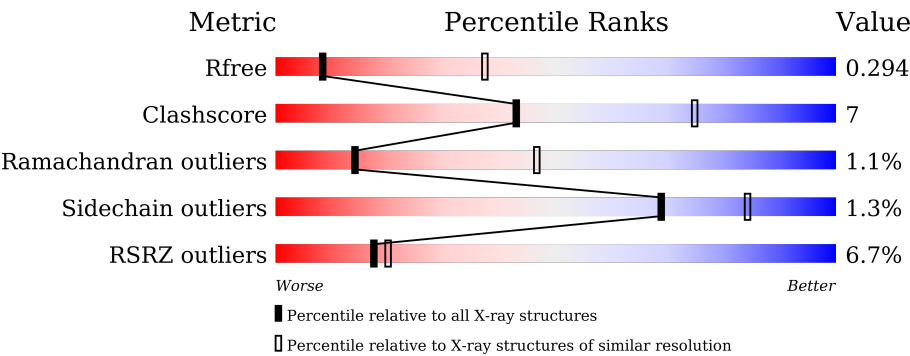
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.37 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	496	<div><div>3%</div><div>68%15%•16%</div></div>
1	B	496	<div><div>3%</div><div>70%12%•17%</div></div>
1	C	496	<div><div>6%</div><div>68%15%•16%</div></div>
1	D	496	<div><div>3%</div><div>69%14%17%</div></div>
1	E	496	<div><div>4%</div><div>67%16%•16%</div></div>
1	F	496	<div><div>5%</div><div>67%14%•18%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	496	<div><div></div><div>7%</div><div>70%</div><div>14%</div><div>•</div><div>16%</div></div>
1	H	496	<div><div></div><div>7%</div><div>68%</div><div>15%</div><div>•</div><div>16%</div></div>
1	I	496	<div><div></div><div>9%</div><div>66%</div><div>15%</div><div>•</div><div>18%</div></div>
1	J	496	<div><div></div><div>7%</div><div>68%</div><div>15%</div><div>•</div><div>16%</div></div>



## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 32368 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	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	B	410	Total	C	N	O	S	0	0	0
			3213	2042	540	612	19			
1	C	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	D	410	Total	C	N	O	S	0	0	0
			3216	2044	541	613	18			
1	E	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	F	407	Total	C	N	O	S	0	0	0
			3194	2031	536	609	18			
1	G	418	Total	C	N	O	S	0	0	0
			3274	2080	550	625	19			
1	H	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	I	405	Total	C	N	O	S	0	0	0
			3181	2025	534	604	18			
1	J	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP Q9W9C6
A	376	VAL	MET	conflict	UNP Q9W9C6
B	-2	MET	-	initiating methionine	UNP Q9W9C6
B	376	VAL	MET	conflict	UNP Q9W9C6
C	-2	MET	-	initiating methionine	UNP Q9W9C6
C	376	VAL	MET	conflict	UNP Q9W9C6
D	-2	MET	-	initiating methionine	UNP Q9W9C6
D	376	VAL	MET	conflict	UNP Q9W9C6
E	-2	MET	-	initiating methionine	UNP Q9W9C6

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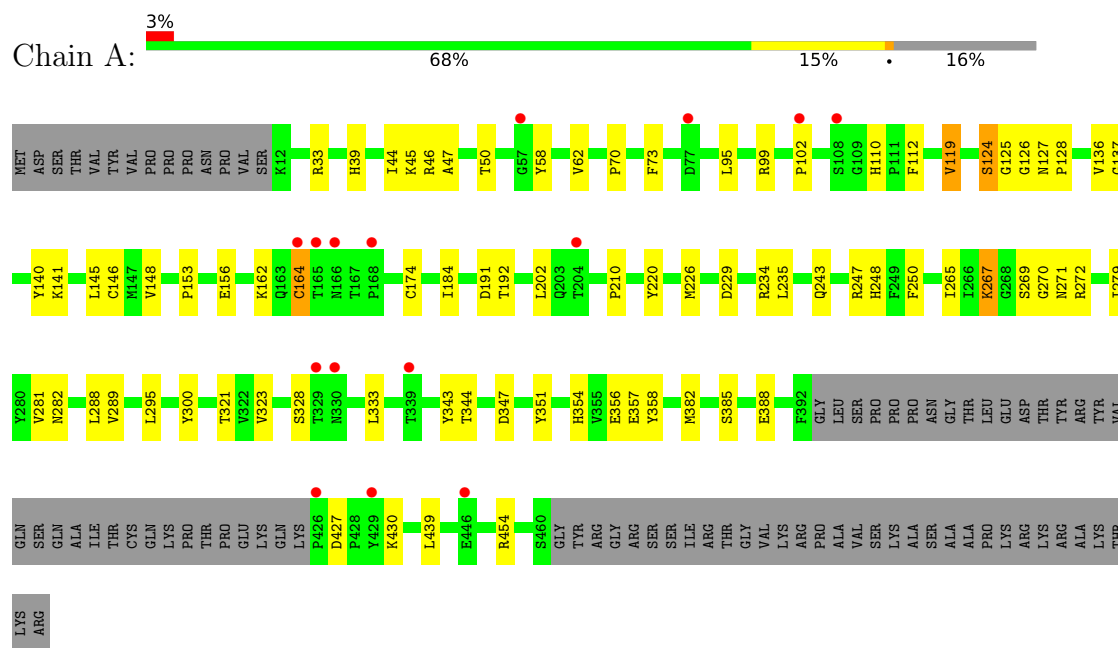
Chain	Residue	Modelled	Actual	Comment	Reference
E	376	VAL	MET	conflict	UNP Q9W9C6
F	-2	MET	-	initiating methionine	UNP Q9W9C6
F	376	VAL	MET	conflict	UNP Q9W9C6
G	-2	MET	-	initiating methionine	UNP Q9W9C6
G	376	VAL	MET	conflict	UNP Q9W9C6
H	-2	MET	-	initiating methionine	UNP Q9W9C6
H	376	VAL	MET	conflict	UNP Q9W9C6
I	-2	MET	-	initiating methionine	UNP Q9W9C6
I	376	VAL	MET	conflict	UNP Q9W9C6
J	-2	MET	-	initiating methionine	UNP Q9W9C6
J	376	VAL	MET	conflict	UNP Q9W9C6



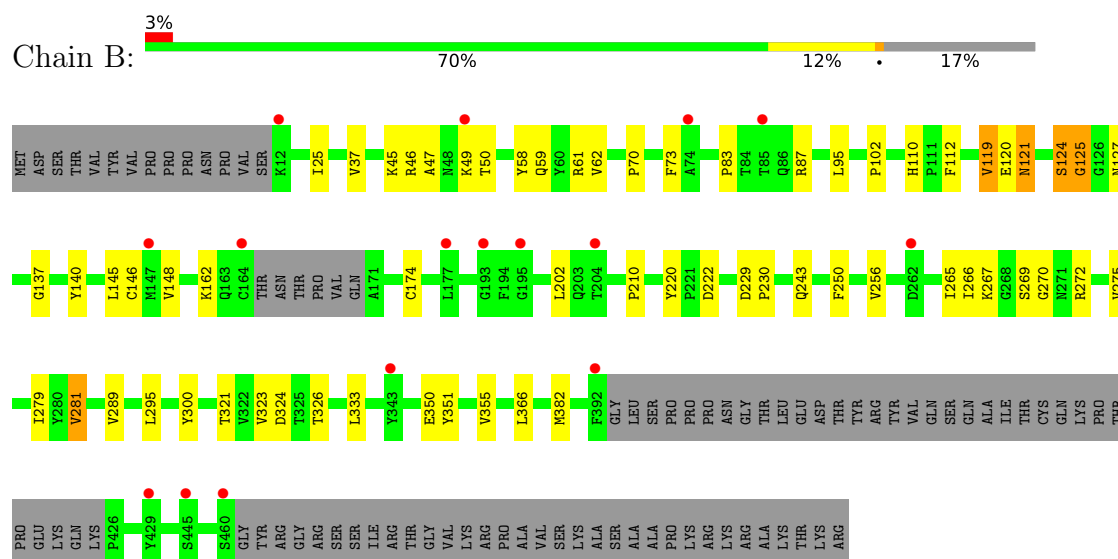
### 3 Residue-property plots

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

#### • Molecule 1: Major capsid protein L1

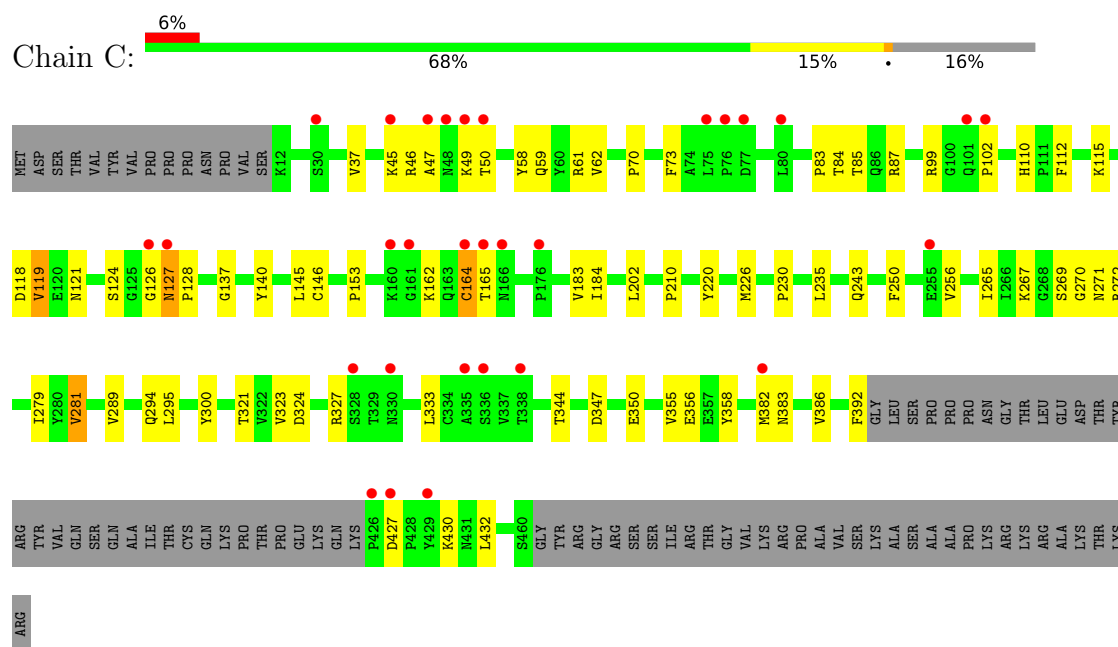


#### • Molecule 1: Major capsid protein L1

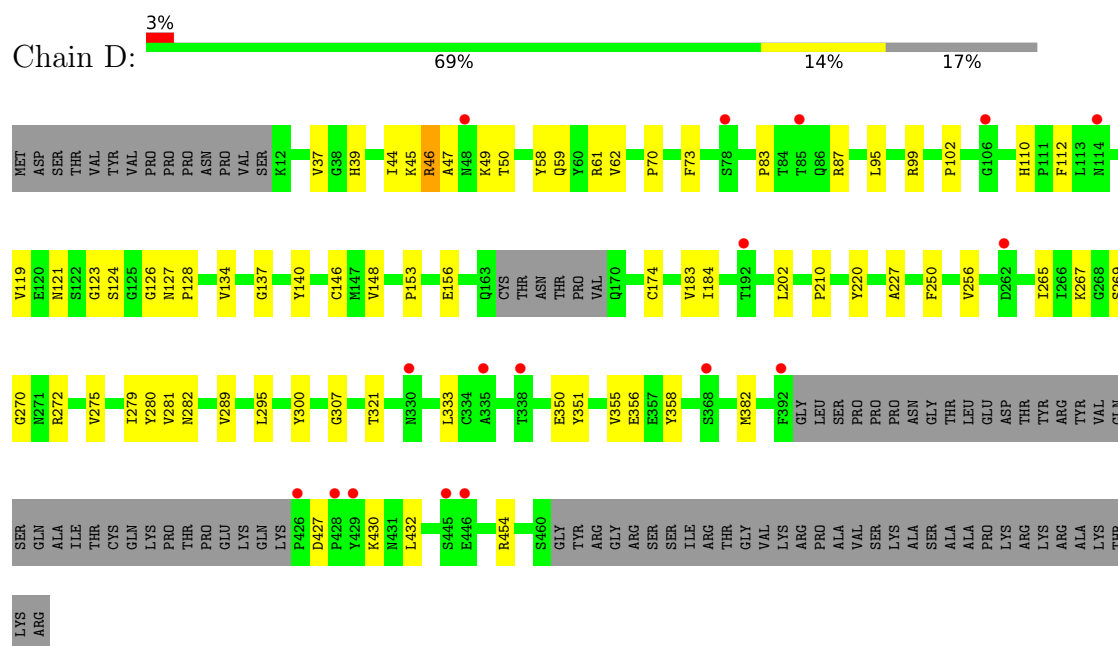




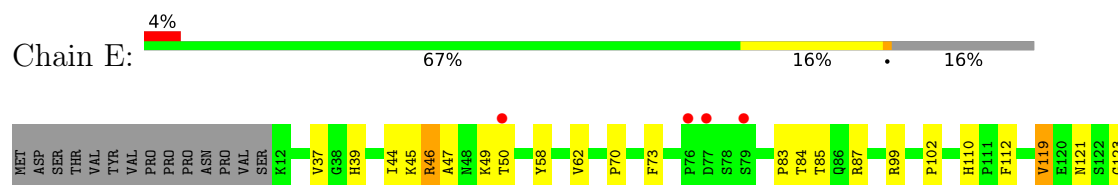
- Molecule 1: Major capsid protein L1



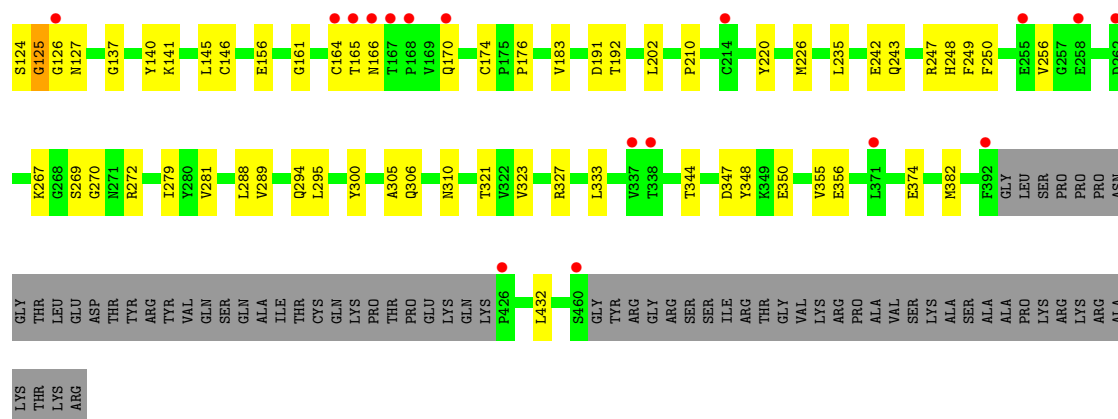
- Molecule 1: Major capsid protein L1



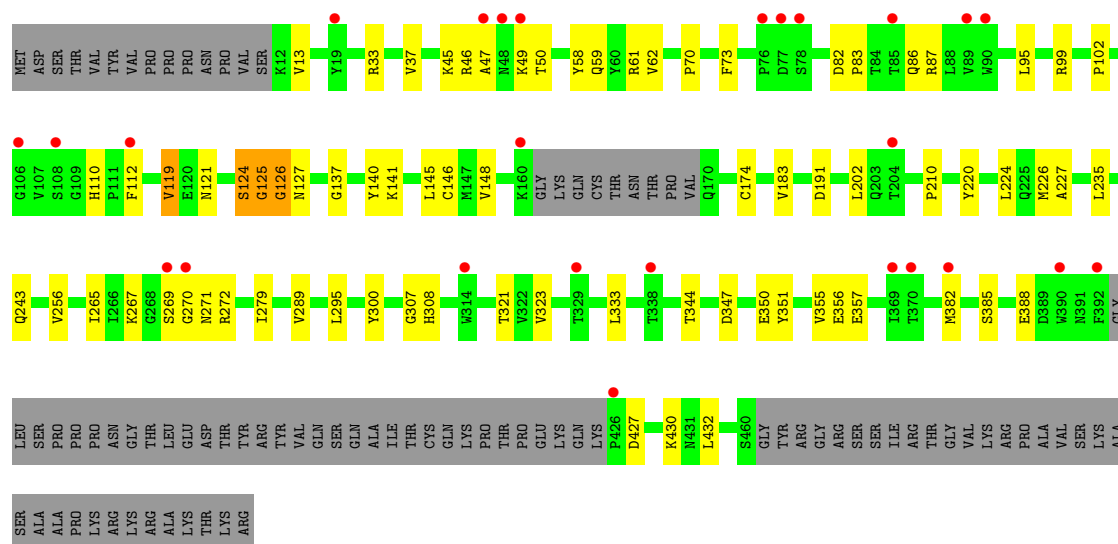
- Molecule 1: Major capsid protein L1



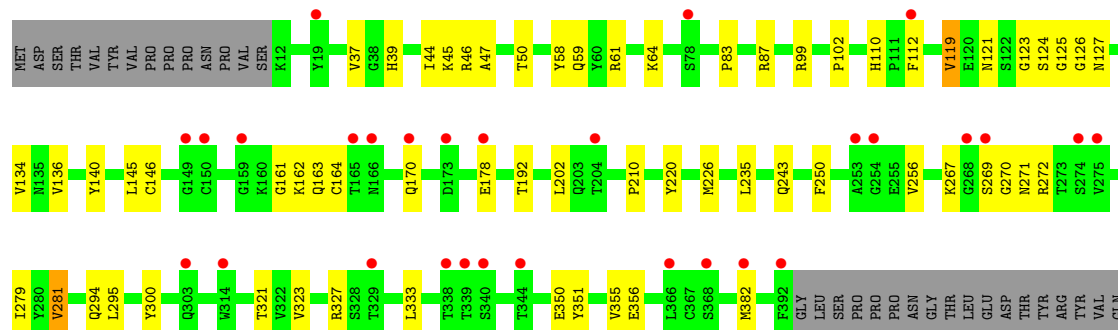




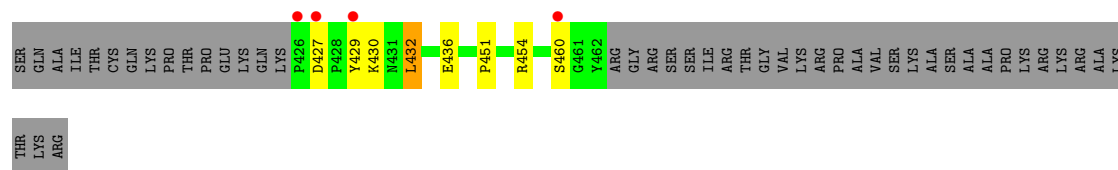
• Molecule 1: Major capsid protein L1



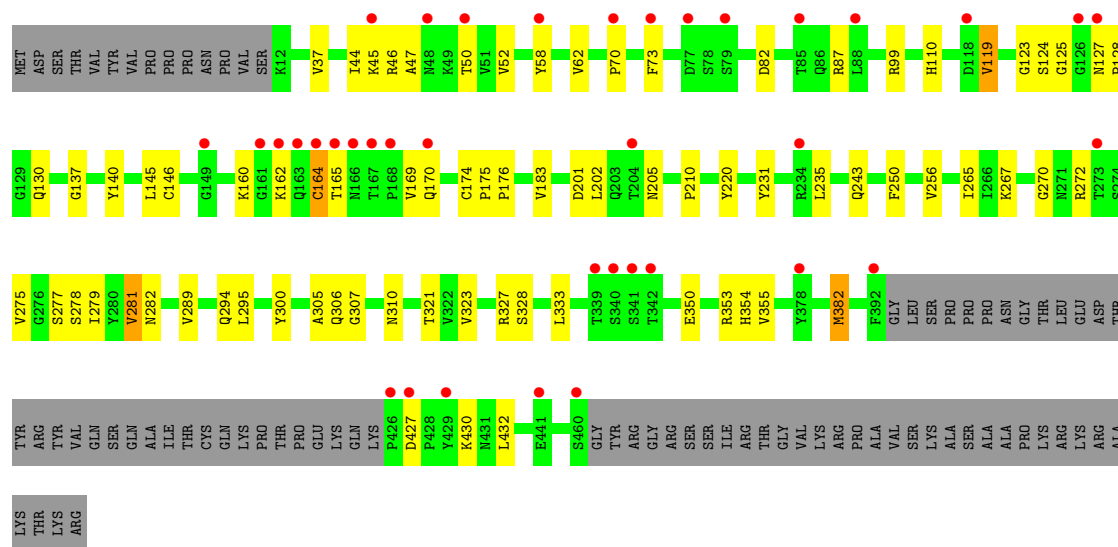
• Molecule 1: Major capsid protein L1



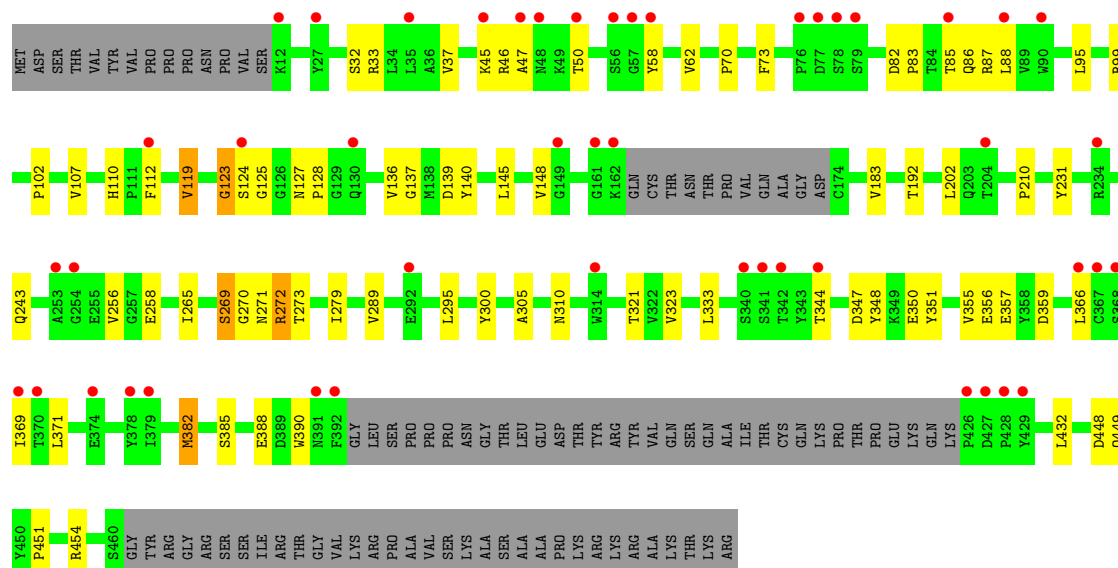




• Molecule 1: Major capsid protein L1

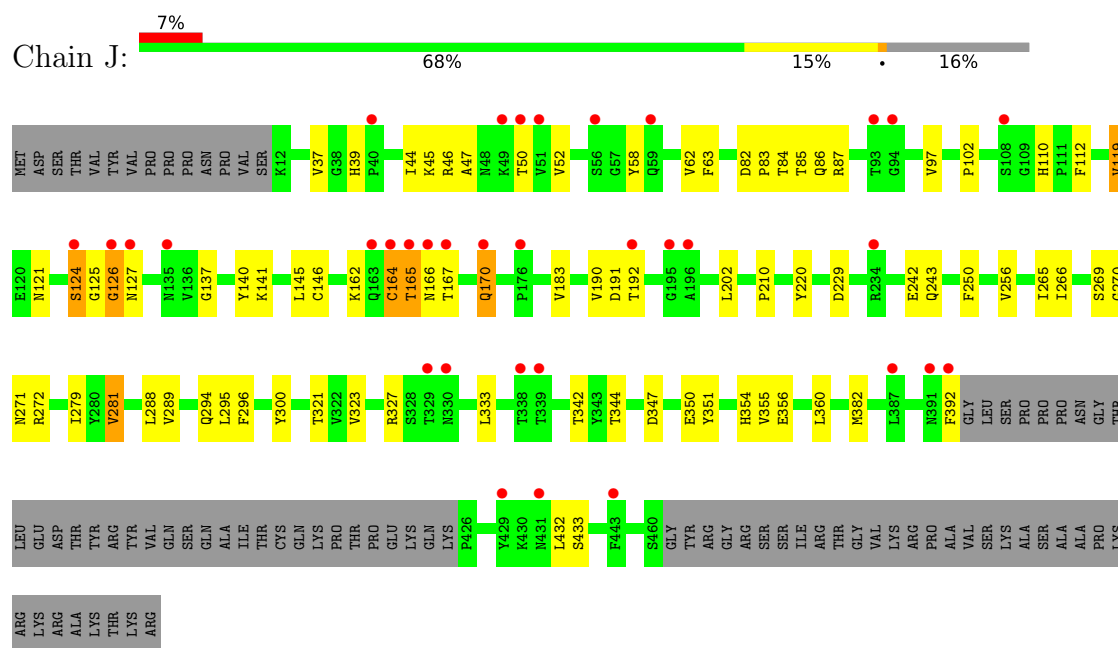


• Molecule 1: Major capsid protein L1



• Molecule 1: Major capsid protein L1







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	308.96Å 106.66Å 198.71Å 90.00° 125.96° 90.00°	Depositor
Resolution (Å)	33.88 – 3.37 33.88 – 3.37	Depositor EDS
% Data completeness (in resolution range)	94.4 (33.88-3.37) 94.4 (33.88-3.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.256 , 0.294 0.256 , 0.294	Depositor DCC
$R_{free}$ test set	3592 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.6	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 22.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	32368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.26	0/3342	0.48	0/4544
1	B	0.26	0/3295	0.47	0/4476
1	C	0.25	0/3342	0.46	0/4544
1	D	0.26	0/3298	0.46	0/4480
1	E	0.25	0/3342	0.46	0/4544
1	F	0.25	0/3276	0.46	0/4452
1	G	0.25	0/3359	0.46	0/4567
1	H	0.26	0/3342	0.47	0/4544
1	I	0.26	0/3263	0.47	0/4433
1	J	0.25	0/3342	0.46	0/4544
All	All	0.25	0/33201	0.47	0/45128

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
1	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	125	GLY	Peptide
1	H	123	GLY	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	3258	0	3150	61	0
1	B	3213	0	3105	49	0
1	C	3258	0	3150	54	0
1	D	3216	0	3108	57	0
1	E	3258	0	3150	58	0
1	F	3194	0	3084	57	0
1	G	3274	0	3162	51	0
1	H	3258	0	3150	49	0
1	I	3181	0	3080	54	0
1	J	3258	0	3150	52	0
All	All	32368	0	31289	430	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 7.

All (430) 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:D:119:VAL:HG11	1:D:280:TYR:HE1	1.43	0.83
1:D:350:GLU:HB2	1:E:279:ILE:HD13	1.59	0.83
1:D:279:ILE:HD13	1:G:350:GLU:HB2	1.65	0.78
1:H:350:GLU:HB2	1:I:279:ILE:HD13	1.66	0.78
1:I:83:PRO:O	1:I:87:ARG:NH1	2.15	0.78
1:D:269:SER:HB3	1:J:342:THR:HG21	1.66	0.77
1:B:279:ILE:HD13	1:F:350:GLU:HB2	1.67	0.76
1:D:295:LEU:O	1:D:300:TYR:OH	2.05	0.75
1:G:460:SER:O	1:H:130:GLN:NE2	2.19	0.75
1:C:350:GLU:HB2	1:J:279:ILE:HD13	1.69	0.74
1:E:295:LEU:O	1:E:300:TYR:OH	2.05	0.74
1:B:83:PRO:O	1:B:87:ARG:NH1	2.20	0.74
1:I:270:GLY:O	1:I:272:ARG:N	2.20	0.74
1:C:279:ILE:HD13	1:E:350:GLU:HB2	1.69	0.73
1:D:256:VAL:HA	1:D:279:ILE:HD11	1.71	0.73
1:A:272:ARG:HD2	1:B:112:PHE:HE1	1.54	0.72
1:A:279:ILE:HD13	1:B:350:GLU:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:O	1:A:300:TYR:OH	2.06	0.72
1:I:295:LEU:O	1:I:300:TYR:OH	2.07	0.72
1:G:279:ILE:HD13	1:J:350:GLU:HB2	1.73	0.70
1:F:83:PRO:O	1:F:87:ARG:NH1	2.24	0.69
1:B:295:LEU:O	1:B:300:TYR:OH	2.10	0.69
1:C:295:LEU:O	1:C:300:TYR:OH	2.09	0.68
1:F:272:ARG:HD2	1:I:112:PHE:HE1	1.57	0.68
1:G:272:ARG:HD2	1:J:112:PHE:HE1	1.58	0.68
1:H:250:PHE:HB2	1:H:281:VAL:HG12	1.76	0.68
1:J:256:VAL:HA	1:J:279:ILE:HD11	1.74	0.67
1:J:164:CYS:O	1:J:166:ASN:N	2.25	0.67
1:J:45:LYS:HB3	1:J:50:THR:HA	1.77	0.67
1:J:250:PHE:HB2	1:J:281:VAL:HG12	1.75	0.67
1:E:83:PRO:O	1:E:87:ARG:NH1	2.26	0.67
1:E:256:VAL:HA	1:E:279:ILE:HD11	1.77	0.66
1:C:250:PHE:HB2	1:C:281:VAL:HG12	1.78	0.66
1:H:256:VAL:HG13	1:H:279:ILE:HD11	1.78	0.65
1:C:256:VAL:HA	1:C:279:ILE:HD11	1.77	0.65
1:B:45:LYS:HB3	1:B:50:THR:HA	1.78	0.65
1:G:256:VAL:HA	1:G:279:ILE:HD11	1.79	0.65
1:A:99:ARG:NH2	1:A:356:GLU:OE1	2.30	0.65
1:C:137:GLY:H	1:J:119:VAL:HG13	1.62	0.65
1:C:112:PHE:HE1	1:J:272:ARG:HD2	1.61	0.64
1:A:202:LEU:HB3	1:B:333:LEU:HD22	1.80	0.63
1:A:333:LEU:HD22	1:H:202:LEU:HB3	1.80	0.63
1:G:269:SER:OG	1:G:270:GLY:N	2.32	0.62
1:F:269:SER:OG	1:F:270:GLY:N	2.32	0.62
1:F:279:ILE:HD13	1:I:350:GLU:HB2	1.80	0.62
1:F:45:LYS:HB3	1:F:50:THR:HA	1.80	0.62
1:D:124:SER:OG	1:D:272:ARG:NE	2.33	0.62
1:A:269:SER:OG	1:A:270:GLY:N	2.32	0.62
1:F:295:LEU:O	1:F:300:TYR:OH	2.16	0.62
1:A:267:LYS:NZ	1:E:374:GLU:OE1	2.29	0.61
1:C:110:HIS:HB2	1:C:210:PRO:HA	1.81	0.61
1:B:222:ASP:OD2	1:F:33:ARG:NH1	2.34	0.61
1:B:250:PHE:HB2	1:B:281:VAL:HG12	1.83	0.61
1:C:83:PRO:O	1:C:87:ARG:NH1	2.33	0.61
1:D:250:PHE:HB2	1:D:281:VAL:HG13	1.82	0.61
1:H:62:VAL:HG22	1:H:321:THR:HG23	1.81	0.61
1:A:45:LYS:HB3	1:A:50:THR:HA	1.82	0.61
1:F:99:ARG:NH2	1:F:356:GLU:OE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:SER:OG	1:C:270:GLY:N	2.34	0.60
1:D:202:LEU:HB3	1:G:333:LEU:HD22	1.82	0.60
1:J:269:SER:OG	1:J:270:GLY:N	2.34	0.60
1:J:183:VAL:HG11	1:J:432:LEU:HD13	1.82	0.60
1:F:183:VAL:HG11	1:F:432:LEU:HD13	1.82	0.60
1:H:45:LYS:HB3	1:H:50:THR:HA	1.84	0.59
1:C:272:ARG:HD2	1:E:112:PHE:HE1	1.68	0.59
1:E:45:LYS:HB3	1:E:50:THR:HA	1.84	0.59
1:B:256:VAL:HA	1:B:279:ILE:HD11	1.85	0.58
1:F:33:ARG:HD2	1:F:357:GLU:OE2	2.03	0.58
1:G:45:LYS:HB3	1:G:50:THR:HA	1.86	0.58
1:F:145:LEU:HG	1:F:323:VAL:HB	1.86	0.58
1:E:62:VAL:HG22	1:E:321:THR:HG23	1.86	0.57
1:C:333:LEU:HD22	1:J:202:LEU:HB3	1.86	0.57
1:J:110:HIS:HB2	1:J:210:PRO:HA	1.86	0.57
1:G:202:LEU:HB3	1:J:333:LEU:HD22	1.87	0.57
1:A:141:LYS:NZ	1:A:191:ASP:OD2	2.25	0.57
1:F:110:HIS:HB2	1:F:210:PRO:HA	1.86	0.57
1:G:46:ARG:HD3	1:G:47:ALA:HB2	1.87	0.57
1:H:427:ASP:HB3	1:H:430:LYS:HG3	1.87	0.57
1:D:110:HIS:HB2	1:D:210:PRO:HA	1.87	0.57
1:E:141:LYS:NZ	1:E:191:ASP:OD2	2.29	0.57
1:F:202:LEU:HB3	1:I:333:LEU:HD22	1.86	0.57
1:I:269:SER:O	1:I:273:THR:HG22	2.05	0.57
1:G:295:LEU:O	1:G:300:TYR:OH	2.15	0.56
1:A:119:VAL:HG13	1:B:137:GLY:H	1.69	0.56
1:C:45:LYS:HB3	1:C:50:THR:HA	1.86	0.56
1:D:119:VAL:HG11	1:D:280:TYR:CE1	2.33	0.56
1:F:13:VAL:O	1:I:449:GLN:NE2	2.37	0.56
1:F:256:VAL:HA	1:F:279:ILE:HD11	1.87	0.56
1:I:123:GLY:O	1:I:125:GLY:HA3	2.05	0.55
1:E:99:ARG:NH2	1:E:356:GLU:OE1	2.39	0.55
1:A:110:HIS:HB2	1:A:210:PRO:HA	1.89	0.55
1:A:220:TYR:CG	1:B:102:PRO:HG3	2.42	0.55
1:A:70:PRO:HA	1:A:73:PHE:HB2	1.88	0.55
1:E:110:HIS:HB2	1:E:210:PRO:HA	1.89	0.55
1:C:85:THR:H	1:C:392:PHE:HE2	1.54	0.54
1:C:272:ARG:HD2	1:E:112:PHE:CE1	2.42	0.54
1:D:62:VAL:HG22	1:D:321:THR:HG23	1.90	0.54
1:G:83:PRO:O	1:G:87:ARG:NH1	2.40	0.54
1:C:220:TYR:CG	1:E:102:PRO:HG3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:45:LYS:HB3	1:I:50:THR:HA	1.89	0.54
1:B:119:VAL:HG13	1:F:137:GLY:H	1.73	0.54
1:B:272:ARG:HD2	1:F:112:PHE:HE1	1.73	0.54
1:D:99:ARG:NH2	1:D:356:GLU:OE1	2.41	0.54
1:F:272:ARG:HD2	1:I:112:PHE:CE1	2.41	0.53
1:G:161:GLY:HA2	1:G:178:GLU:OE2	2.08	0.53
1:F:265:ILE:HG22	1:I:110:HIS:HE1	1.72	0.53
1:H:295:LEU:O	1:H:300:TYR:OH	2.22	0.53
1:I:256:VAL:HA	1:I:279:ILE:HD11	1.91	0.53
1:A:46:ARG:NH2	1:A:47:ALA:HB2	2.23	0.53
1:C:59:GLN:OE1	1:C:61:ARG:NH2	2.41	0.53
1:D:39:HIS:HD2	1:D:44:ILE:HD11	1.73	0.53
1:E:124:SER:OG	1:E:125:GLY:N	2.37	0.53
1:G:162:LYS:HD3	1:G:164:CYS:HA	1.91	0.53
1:B:202:LEU:HB3	1:F:333:LEU:HD22	1.90	0.52
1:J:39:HIS:HD2	1:J:44:ILE:HD11	1.73	0.52
1:G:110:HIS:HB2	1:G:210:PRO:HA	1.90	0.52
1:J:83:PRO:O	1:J:87:ARG:NH1	2.41	0.52
1:H:124:SER:HB3	1:H:125:GLY:C	2.30	0.52
1:B:62:VAL:HG22	1:B:321:THR:HG23	1.90	0.52
1:I:269:SER:OG	1:I:270:GLY:N	2.43	0.52
1:A:102:PRO:HG3	1:H:220:TYR:CG	2.45	0.51
1:B:220:TYR:CG	1:F:102:PRO:HG3	2.45	0.51
1:C:145:LEU:HG	1:C:323:VAL:HB	1.91	0.51
1:D:183:VAL:HG11	1:D:432:LEU:HD13	1.92	0.51
1:A:250:PHE:HB2	1:A:281:VAL:HG13	1.91	0.51
1:C:294:GLN:OE1	1:C:327:ARG:NH1	2.38	0.51
1:E:183:VAL:HG11	1:E:432:LEU:HD13	1.93	0.51
1:A:226:MET:HB3	1:A:235:LEU:HG	1.92	0.51
1:C:62:VAL:HG22	1:C:321:THR:HG23	1.93	0.51
1:C:127:ASN:ND2	1:C:128:PRO:HD2	2.25	0.51
1:C:202:LEU:HB3	1:E:333:LEU:HD22	1.91	0.51
1:H:160:LYS:HE3	1:H:201:ASP:HB3	1.91	0.51
1:I:70:PRO:HA	1:I:73:PHE:HB2	1.93	0.51
1:A:427:ASP:HB3	1:A:430:LYS:HG3	1.92	0.51
1:J:141:LYS:NZ	1:J:191:ASP:OD2	2.25	0.51
1:J:146:CYS:HA	1:J:321:THR:O	2.11	0.51
1:B:46:ARG:HD2	1:B:47:ALA:HB2	1.92	0.51
1:D:45:LYS:HB3	1:D:50:THR:HA	1.93	0.50
1:A:137:GLY:H	1:H:119:VAL:HG13	1.75	0.50
1:C:70:PRO:HA	1:C:73:PHE:HB2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:TYR:CG	1:G:102:PRO:HG3	2.46	0.50
1:D:112:PHE:HE1	1:E:272:ARG:HD2	1.75	0.50
1:F:95:LEU:HD22	1:F:148:VAL:HG21	1.94	0.50
1:A:162:LYS:HG3	1:A:164:CYS:H	1.76	0.50
1:A:356:GLU:HB3	1:A:358:TYR:HE2	1.76	0.50
1:D:272:ARG:HD2	1:G:112:PHE:HE1	1.75	0.50
1:G:220:TYR:CG	1:J:102:PRO:HG3	2.46	0.50
1:D:265:ILE:HG22	1:G:110:HIS:HE1	1.76	0.50
1:F:141:LYS:NZ	1:F:191:ASP:OD2	2.32	0.50
1:A:62:VAL:HG22	1:A:321:THR:HG23	1.92	0.50
1:B:272:ARG:HD2	1:F:112:PHE:CE1	2.46	0.50
1:F:307:GLY:HA2	1:I:454:ARG:NH1	2.27	0.50
1:H:110:HIS:HB2	1:H:210:PRO:HA	1.93	0.50
1:J:85:THR:H	1:J:392:PHE:HE2	1.60	0.50
1:J:141:LYS:HE3	1:J:242:GLU:HB3	1.94	0.50
1:G:427:ASP:HB3	1:G:430:LYS:HG3	1.94	0.49
1:C:119:VAL:HG13	1:E:137:GLY:H	1.77	0.49
1:D:333:LEU:HD22	1:E:202:LEU:HB3	1.94	0.49
1:F:62:VAL:HG22	1:F:321:THR:HG23	1.92	0.49
1:B:37:VAL:HG22	1:B:355:VAL:HG12	1.95	0.49
1:D:153:PRO:HG2	1:D:184:ILE:HB	1.95	0.49
1:G:250:PHE:HB2	1:G:281:VAL:HG12	1.93	0.49
1:H:333:LEU:HD22	1:I:202:LEU:HB3	1.95	0.49
1:I:183:VAL:HG11	1:I:432:LEU:HD13	1.94	0.49
1:D:127:ASN:HB3	1:D:128:PRO:HD2	1.94	0.49
1:J:62:VAL:HG22	1:J:321:THR:HG23	1.94	0.49
1:D:137:GLY:H	1:E:119:VAL:HG13	1.77	0.48
1:H:46:ARG:HA	1:H:47:ALA:HA	1.54	0.48
1:I:145:LEU:HG	1:I:323:VAL:HB	1.94	0.48
1:E:226:MET:HB3	1:E:235:LEU:HG	1.96	0.48
1:F:308:HIS:NE2	1:I:448:ASP:O	2.46	0.48
1:H:137:GLY:H	1:I:119:VAL:HG13	1.77	0.48
1:B:243:GLN:HA	1:F:289:VAL:O	2.13	0.48
1:C:243:GLN:HA	1:E:289:VAL:O	2.13	0.48
1:H:183:VAL:HG11	1:H:432:LEU:HD13	1.94	0.48
1:C:112:PHE:CE1	1:J:272:ARG:HD2	2.44	0.48
1:C:183:VAL:HG11	1:C:432:LEU:HD13	1.95	0.48
1:F:37:VAL:HG22	1:F:355:VAL:HG12	1.94	0.48
1:A:289:VAL:O	1:H:243:GLN:HA	2.13	0.48
1:C:146:CYS:HA	1:C:321:THR:O	2.14	0.48
1:A:272:ARG:HD2	1:B:112:PHE:CE1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:GLU:HB3	1:C:358:TYR:HE2	1.79	0.48
1:E:145:LEU:HG	1:E:323:VAL:HB	1.96	0.48
1:C:102:PRO:HG3	1:J:220:TYR:CG	2.48	0.48
1:E:140:TYR:CD1	1:E:192:THR:HB	2.48	0.48
1:E:294:GLN:OE1	1:E:327:ARG:NH1	2.39	0.48
1:D:134:VAL:HG13	1:E:123:GLY:HA3	1.94	0.48
1:G:124:SER:OG	1:G:125:GLY:N	2.47	0.47
1:J:294:GLN:OE1	1:J:327:ARG:NH1	2.41	0.47
1:A:145:LEU:HG	1:A:323:VAL:HB	1.96	0.47
1:B:59:GLN:OE1	1:B:61:ARG:NH2	2.47	0.47
1:J:145:LEU:HG	1:J:323:VAL:HB	1.96	0.47
1:D:46:ARG:HA	1:D:47:ALA:HA	1.52	0.47
1:F:427:ASP:HB3	1:F:430:LYS:HG3	1.97	0.47
1:I:110:HIS:HB2	1:I:210:PRO:HA	1.96	0.47
1:A:39:HIS:HD2	1:A:44:ILE:HD11	1.78	0.47
1:B:269:SER:OG	1:B:270:GLY:N	2.46	0.47
1:H:145:LEU:HG	1:H:323:VAL:HB	1.97	0.47
1:B:110:HIS:HB2	1:B:210:PRO:HA	1.97	0.47
1:E:269:SER:OG	1:E:270:GLY:N	2.47	0.47
1:G:119:VAL:HG13	1:J:137:GLY:H	1.80	0.47
1:H:294:GLN:OE1	1:H:327:ARG:NH1	2.42	0.47
1:I:99:ARG:NH2	1:I:356:GLU:OE1	2.47	0.47
1:J:295:LEU:O	1:J:300:TYR:OH	2.22	0.47
1:H:162:LYS:HG3	1:H:164:CYS:H	1.79	0.47
1:C:99:ARG:NE	1:C:324:ASP:OD2	2.48	0.47
1:D:146:CYS:HA	1:D:321:THR:O	2.15	0.47
1:G:64:LYS:HD3	1:G:436:GLU:OE2	2.15	0.47
1:D:83:PRO:O	1:D:87:ARG:NH1	2.49	0.46
1:G:58:TYR:CE1	1:G:140:TYR:HB2	2.50	0.46
1:B:49:LYS:HA	1:B:49:LYS:NZ	2.30	0.46
1:C:37:VAL:HG22	1:C:355:VAL:HG12	1.97	0.46
1:F:126:GLY:HA3	1:F:127:ASN:HA	1.60	0.46
1:J:46:ARG:HA	1:J:47:ALA:HA	1.51	0.46
1:B:120:GLU:HB3	1:B:121:ASN:OD1	2.16	0.46
1:I:87:ARG:HG3	1:I:390:TRP:CD2	2.50	0.46
1:A:112:PHE:CZ	1:H:275:VAL:HA	2.51	0.46
1:F:46:ARG:HA	1:F:47:ALA:HA	1.54	0.46
1:E:46:ARG:HA	1:E:47:ALA:HA	1.53	0.46
1:J:44:ILE:HB	1:J:52:VAL:HB	1.98	0.46
1:B:46:ARG:HA	1:B:47:ALA:HA	1.59	0.46
1:D:307:GLY:HA2	1:G:454:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:CYS:HA	1:F:321:THR:O	2.16	0.46
1:G:37:VAL:HG13	1:G:355:VAL:HG12	1.98	0.46
1:A:46:ARG:HA	1:A:47:ALA:HA	1.53	0.46
1:A:288:LEU:HD22	1:H:243:GLN:HB2	1.98	0.46
1:I:33:ARG:HD2	1:I:357:GLU:OE2	2.15	0.46
1:A:265:ILE:HG22	1:B:110:HIS:HE1	1.80	0.46
1:C:49:LYS:NZ	1:C:49:LYS:HA	2.30	0.46
1:I:86:GLN:HA	1:I:369:ILE:O	2.16	0.46
1:I:385:SER:HA	1:I:388:GLU:HB2	1.97	0.46
1:C:427:ASP:HB3	1:C:430:LYS:HG3	1.98	0.46
1:I:85:THR:O	1:I:371:LEU:N	2.42	0.46
1:C:243:GLN:HB2	1:E:288:LEU:HD22	1.98	0.46
1:H:44:ILE:HB	1:H:52:VAL:HB	1.98	0.46
1:H:70:PRO:HA	1:H:73:PHE:HB2	1.97	0.46
1:A:156:GLU:N	1:A:220:TYR:O	2.38	0.45
1:B:174:CYS:HB2	1:F:351:TYR:CD2	2.51	0.45
1:G:272:ARG:HD2	1:J:112:PHE:CE1	2.45	0.45
1:A:126:GLY:HA3	1:A:127:ASN:HA	1.76	0.45
1:D:102:PRO:HG3	1:E:220:TYR:CG	2.51	0.45
1:H:37:VAL:HG22	1:H:355:VAL:HG12	1.98	0.45
1:H:235:LEU:HB2	1:H:306:GLN:HE21	1.81	0.45
1:I:58:TYR:CE1	1:I:140:TYR:HB2	2.52	0.45
1:G:123:GLY:O	1:G:124:SER:HB3	2.17	0.45
1:I:82:ASP:O	1:I:86:GLN:HB2	2.16	0.45
1:C:118:ASP:HB2	1:J:121:ASN:HD21	1.82	0.45
1:D:37:VAL:HG22	1:D:355:VAL:HG12	1.98	0.45
1:F:226:MET:HB3	1:F:235:LEU:HG	1.98	0.45
1:D:112:PHE:CE1	1:E:272:ARG:HD2	2.52	0.45
1:F:59:GLN:OE1	1:F:61:ARG:NH2	2.49	0.45
1:G:99:ARG:NH2	1:G:356:GLU:OE1	2.50	0.45
1:G:145:LEU:HG	1:G:323:VAL:HB	1.98	0.45
1:A:99:ARG:HA	1:A:99:ARG:HD2	1.87	0.45
1:B:146:CYS:HA	1:B:321:THR:O	2.17	0.45
1:D:126:GLY:HA3	1:D:127:ASN:HA	1.72	0.45
1:E:84:THR:O	1:E:85:THR:OG1	2.33	0.45
1:J:333:LEU:HB2	1:J:351:TYR:HB2	1.98	0.45
1:A:328:SER:HA	1:A:354:HIS:CE1	2.51	0.45
1:A:243:GLN:HA	1:B:289:VAL:O	2.16	0.45
1:B:37:VAL:HG13	1:B:355:VAL:HG12	1.99	0.45
1:F:119:VAL:O	1:I:136:VAL:HA	2.16	0.45
1:H:146:CYS:HA	1:H:321:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ILE:HG22	1:E:110:HIS:HE1	1.82	0.44
1:G:46:ARG:HA	1:G:47:ALA:HA	1.53	0.44
1:J:124:SER:HA	1:J:125:GLY:HA2	1.50	0.44
1:A:58:TYR:CE1	1:A:140:TYR:HB2	2.53	0.44
1:C:153:PRO:HG2	1:C:184:ILE:HB	1.98	0.44
1:F:124:SER:HA	1:F:125:GLY:HA2	1.49	0.44
1:H:270:GLY:O	1:H:272:ARG:N	2.47	0.44
1:I:95:LEU:HD22	1:I:148:VAL:HG21	2.00	0.44
1:A:112:PHE:HZ	1:H:275:VAL:HA	1.80	0.44
1:A:112:PHE:HE1	1:H:272:ARG:HD2	1.83	0.44
1:A:454:ARG:NH1	1:H:307:GLY:HA2	2.32	0.44
1:C:344:THR:OG1	1:C:347:ASP:OD2	2.35	0.44
1:D:272:ARG:HA	1:D:272:ARG:HD3	1.66	0.44
1:F:58:TYR:CE1	1:F:140:TYR:HB2	2.53	0.44
1:F:265:ILE:HG22	1:I:110:HIS:CE1	2.52	0.44
1:G:146:CYS:HA	1:G:321:THR:O	2.17	0.44
1:J:58:TYR:CE1	1:J:140:TYR:HB2	2.53	0.44
1:A:153:PRO:HG2	1:A:184:ILE:HB	1.98	0.44
1:B:95:LEU:HD22	1:B:148:VAL:HG21	1.98	0.44
1:C:289:VAL:O	1:J:243:GLN:HA	2.17	0.44
1:E:250:PHE:HB2	1:E:281:VAL:CG1	2.47	0.44
1:F:224:LEU:HD13	1:I:359:ASP:HB2	2.00	0.44
1:H:289:VAL:O	1:I:243:GLN:HA	2.17	0.44
1:I:46:ARG:HA	1:I:47:ALA:HA	1.54	0.44
1:D:351:TYR:CD2	1:E:174:CYS:HB2	2.53	0.44
1:E:126:GLY:HA3	1:E:127:ASN:OD1	2.18	0.44
1:H:58:TYR:CE1	1:H:140:TYR:HB2	2.53	0.44
1:H:328:SER:HA	1:H:354:HIS:CE1	2.52	0.44
1:B:49:LYS:HA	1:B:49:LYS:HZ2	1.81	0.44
1:B:265:ILE:HG22	1:F:110:HIS:HE1	1.83	0.44
1:E:58:TYR:CE1	1:E:140:TYR:HB2	2.53	0.44
1:E:146:CYS:HA	1:E:321:THR:O	2.18	0.44
1:A:95:LEU:HD22	1:A:148:VAL:HG21	1.99	0.44
1:A:146:CYS:HA	1:A:321:THR:O	2.18	0.44
1:D:119:VAL:HG12	1:G:136:VAL:HA	2.00	0.44
1:C:115:LYS:NZ	1:J:121:ASN:OD1	2.29	0.44
1:D:123:GLY:HA3	1:G:134:VAL:HG13	2.00	0.44
1:A:344:THR:OG1	1:A:347:ASP:OD2	2.36	0.43
1:A:385:SER:HA	1:A:388:GLU:HB2	1.99	0.43
1:D:272:ARG:HD2	1:G:112:PHE:CE1	2.53	0.43
1:B:324:ASP:OD1	1:B:326:THR:OG1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:GLY:HA3	1:C:127:ASN:OD1	2.18	0.43
1:I:107:VAL:HG12	1:I:139:ASP:HB3	1.99	0.43
1:J:37:VAL:HG22	1:J:355:VAL:HG12	2.00	0.43
1:A:343:TYR:HE2	1:H:205:ASN:HB2	1.84	0.43
1:C:58:TYR:CE1	1:C:140:TYR:HB2	2.54	0.43
1:G:243:GLN:HA	1:J:289:VAL:O	2.17	0.43
1:D:58:TYR:CE1	1:D:140:TYR:HB2	2.53	0.43
1:D:95:LEU:HD22	1:D:148:VAL:HG21	2.01	0.43
1:E:37:VAL:HG22	1:E:355:VAL:HG12	2.00	0.43
1:F:119:VAL:HG13	1:I:137:GLY:H	1.84	0.43
1:I:62:VAL:HG22	1:I:321:THR:HG23	1.99	0.43
1:D:289:VAL:O	1:E:243:GLN:HA	2.18	0.43
1:F:220:TYR:CG	1:I:102:PRO:HG3	2.54	0.43
1:D:121:ASN:OD1	1:D:121:ASN:N	2.52	0.43
1:E:39:HIS:HD2	1:E:44:ILE:HD11	1.84	0.43
1:E:344:THR:OG1	1:E:347:ASP:OD2	2.36	0.43
1:G:140:TYR:CG	1:G:192:THR:HB	2.54	0.43
1:J:354:HIS:NE2	1:J:356:GLU:OE2	2.49	0.43
1:C:99:ARG:HA	1:C:99:ARG:HD2	1.91	0.42
1:F:344:THR:OG1	1:F:347:ASP:OD2	2.37	0.42
1:I:88:LEU:HB3	1:I:366:LEU:HD11	2.01	0.42
1:A:33:ARG:HD2	1:A:357:GLU:OE2	2.20	0.42
1:I:127:ASN:HB3	1:I:128:PRO:HD2	2.00	0.42
1:B:124:SER:HB3	1:B:125:GLY:HA2	2.01	0.42
1:D:156:GLU:N	1:D:220:TYR:O	2.38	0.42
1:E:161:GLY:N	1:E:176:PRO:O	2.50	0.42
1:H:277:SER:OG	1:H:279:ILE:HD12	2.19	0.42
1:B:25:ILE:HB	1:B:366:LEU:HB3	2.02	0.42
1:E:124:SER:OG	1:E:272:ARG:NE	2.52	0.42
1:F:82:ASP:O	1:F:86:GLN:HB2	2.19	0.42
1:I:305:ALA:HB3	1:I:310:ASN:HA	2.00	0.42
1:C:84:THR:O	1:C:85:THR:OG1	2.32	0.42
1:F:243:GLN:HA	1:I:289:VAL:O	2.19	0.42
1:C:110:HIS:HE1	1:J:265:ILE:HG22	1.84	0.42
1:D:454:ARG:NH1	1:E:306:GLN:OE1	2.52	0.42
1:E:70:PRO:HA	1:E:73:PHE:HB2	2.01	0.42
1:J:82:ASP:O	1:J:86:GLN:HB2	2.19	0.42
1:A:136:VAL:HA	1:H:119:VAL:O	2.20	0.42
1:A:229:ASP:OD2	1:A:234:ARG:NH1	2.52	0.42
1:C:99:ARG:NH2	1:C:356:GLU:OE1	2.53	0.42
1:C:226:MET:HB3	1:C:235:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ARG:HA	1:E:46:ARG:HD2	1.87	0.42
1:F:70:PRO:HA	1:F:73:PHE:HB2	2.02	0.42
1:G:226:MET:HB3	1:G:235:LEU:HG	2.02	0.42
1:G:429:TYR:HA	1:G:432:LEU:HD12	2.02	0.42
1:H:353:ARG:NH2	1:I:258:GLU:OE1	2.47	0.42
1:A:439:LEU:HD23	1:A:439:LEU:HA	1.91	0.42
1:B:266:ILE:HD13	1:I:348:TYR:OH	2.19	0.42
1:D:99:ARG:HA	1:D:99:ARG:HD2	1.89	0.42
1:G:121:ASN:OD1	1:G:121:ASN:N	2.53	0.42
1:C:46:ARG:HA	1:C:47:ALA:HA	1.55	0.42
1:F:121:ASN:OD1	1:F:121:ASN:N	2.52	0.42
1:F:174:CYS:HB2	1:I:351:TYR:CD2	2.54	0.42
1:I:344:THR:OG1	1:I:347:ASP:OD2	2.38	0.42
1:A:247:ARG:HG3	1:A:248:HIS:CD2	2.55	0.42
1:B:46:ARG:HH21	1:B:46:ARG:HG3	1.85	0.42
1:B:145:LEU:HG	1:B:323:VAL:HB	2.02	0.42
1:J:344:THR:OG1	1:J:347:ASP:OD2	2.37	0.42
1:D:227:ALA:O	1:G:451:PRO:HG3	2.20	0.41
1:H:110:HIS:HE1	1:I:265:ILE:HG22	1.85	0.41
1:H:231:TYR:CE2	1:H:382:MET:HA	2.55	0.41
1:H:305:ALA:HB3	1:H:310:ASN:HA	2.02	0.41
1:A:153:PRO:HG3	1:A:321:THR:OG1	2.20	0.41
1:A:250:PHE:HB2	1:A:281:VAL:CG1	2.49	0.41
1:C:383:ASN:HB3	1:C:386:VAL:HG23	2.01	0.41
1:E:141:LYS:HE3	1:E:242:GLU:HB3	2.03	0.41
1:J:63:PHE:CG	1:J:360:LEU:HD11	2.55	0.41
1:J:126:GLY:HA3	1:J:127:ASN:HA	1.73	0.41
1:C:121:ASN:OD1	1:C:121:ASN:N	2.54	0.41
1:J:84:THR:O	1:J:85:THR:OG1	2.32	0.41
1:A:140:TYR:CD1	1:A:192:THR:HB	2.56	0.41
1:C:272:ARG:HD3	1:C:272:ARG:HA	1.92	0.41
1:D:275:VAL:HG22	1:G:112:PHE:CZ	2.56	0.41
1:H:175:PRO:HA	1:H:176:PRO:HD3	1.97	0.41
1:A:110:HIS:HE1	1:H:265:ILE:HG22	1.84	0.41
1:C:37:VAL:HG13	1:C:355:VAL:HG12	2.02	0.41
1:F:272:ARG:HD3	1:F:272:ARG:HA	1.93	0.41
1:G:162:LYS:C	1:G:164:CYS:H	2.24	0.41
1:H:99:ARG:HA	1:H:99:ARG:HD2	1.90	0.41
1:H:127:ASN:CG	1:H:128:PRO:HD2	2.40	0.41
1:I:231:TYR:CE2	1:I:382:MET:HA	2.56	0.41
1:B:70:PRO:HA	1:B:73:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:VAL:HG22	1:B:279:ILE:HD11	2.02	0.41
1:E:121:ASN:OD1	1:E:121:ASN:N	2.53	0.41
1:E:170:GLN:H	1:E:170:GLN:HG2	1.50	0.41
1:E:247:ARG:HG3	1:E:248:HIS:CD2	2.56	0.41
1:F:385:SER:HA	1:F:388:GLU:HB2	2.03	0.41
1:D:356:GLU:HB3	1:D:358:TYR:HE2	1.85	0.41
1:B:58:TYR:CE1	1:B:140:TYR:HB2	2.56	0.41
1:B:121:ASN:OD1	1:B:121:ASN:N	2.52	0.41
1:C:162:LYS:HG3	1:C:164:CYS:H	1.86	0.41
1:D:46:ARG:HA	1:D:46:ARG:HD2	1.84	0.41
1:D:275:VAL:HG22	1:G:112:PHE:HZ	1.86	0.41
1:G:39:HIS:HD2	1:G:44:ILE:HD11	1.85	0.41
1:A:124:SER:HB3	1:A:125:GLY:HA3	2.03	0.41
1:A:351:TYR:CD2	1:H:174:CYS:HB2	2.55	0.41
1:D:350:GLU:HB3	1:E:279:ILE:HG21	2.01	0.41
1:E:348:TYR:OH	1:J:266:ILE:HD13	2.20	0.41
1:G:294:GLN:OE1	1:G:327:ARG:NH1	2.46	0.41
1:A:174:CYS:HB2	1:B:351:TYR:CD2	2.55	0.40
1:D:279:ILE:HG21	1:G:350:GLU:HB3	2.02	0.40
1:H:87:ARG:HA	1:H:87:ARG:HD2	1.92	0.40
1:I:140:TYR:CD1	1:I:192:THR:HB	2.56	0.40
1:J:140:TYR:CD1	1:J:192:THR:HB	2.56	0.40
1:J:162:LYS:C	1:J:164:CYS:H	2.24	0.40
1:D:70:PRO:HA	1:D:73:PHE:HB2	2.03	0.40
1:D:267:LYS:HE3	1:D:267:LYS:HB2	1.88	0.40
1:D:427:ASP:HB3	1:D:430:LYS:HG3	2.03	0.40
1:E:99:ARG:HA	1:E:99:ARG:HD2	1.88	0.40
1:E:156:GLU:HG2	1:E:220:TYR:O	2.21	0.40
1:G:37:VAL:HG22	1:G:355:VAL:HG12	2.02	0.40
1:A:267:LYS:HB2	1:A:267:LYS:HZ2	1.86	0.40
1:D:59:GLN:OE1	1:D:61:ARG:NH2	2.54	0.40
1:D:174:CYS:HB2	1:G:351:TYR:CD2	2.56	0.40
1:F:49:LYS:HA	1:F:49:LYS:HD3	1.90	0.40
1:F:227:ALA:O	1:I:451:PRO:HG3	2.21	0.40
1:G:59:GLN:OE1	1:G:61:ARG:NH2	2.54	0.40
1:I:37:VAL:HG13	1:I:355:VAL:HG12	2.03	0.40
1:A:119:VAL:HG13	1:B:137:GLY:N	2.37	0.40
1:A:127:ASN:HB3	1:A:128:PRO:HD2	2.03	0.40
1:B:275:VAL:HA	1:F:112:PHE:HZ	1.87	0.40
1:E:305:ALA:HB3	1:E:310:ASN:HA	2.04	0.40
1:E:119:VAL:HG12	1:E:249:PHE:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:SER:HB3	1:F:272:ARG:NE	2.36	0.40
1:J:97:VAL:O	1:J:296:PHE:HB3	2.21	0.40
1:J:190:VAL:HG21	1:J:323:VAL:HG11	2.03	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	412/496 (83%)	389 (94%)	19 (5%)	4 (1%)	15	49
1	B	404/496 (82%)	385 (95%)	15 (4%)	4 (1%)	15	49
1	C	412/496 (83%)	391 (95%)	15 (4%)	6 (2%)	10	39
1	D	404/496 (82%)	387 (96%)	15 (4%)	2 (0%)	29	63
1	E	412/496 (83%)	390 (95%)	18 (4%)	4 (1%)	15	49
1	F	401/496 (81%)	382 (95%)	15 (4%)	4 (1%)	15	49
1	G	414/496 (84%)	391 (94%)	19 (5%)	4 (1%)	15	49
1	H	412/496 (83%)	393 (95%)	15 (4%)	4 (1%)	15	49
1	I	399/496 (80%)	382 (96%)	12 (3%)	5 (1%)	12	42
1	J	412/496 (83%)	388 (94%)	17 (4%)	7 (2%)	9	36
All	All	4082/4960 (82%)	3878 (95%)	160 (4%)	44 (1%)	14	46

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	382	MET
1	F	126	GLY
1	I	269	SER
1	I	271	ASN

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Mol	Chain	Res	Type
1	J	126	GLY
1	A	271	ASN
1	A	382	MET
1	B	124	SER
1	B	382	MET
1	C	124	SER
1	C	271	ASN
1	D	382	MET
1	E	125	GLY
1	E	382	MET
1	F	124	SER
1	F	271	ASN
1	F	382	MET
1	G	126	GLY
1	G	271	ASN
1	G	382	MET
1	H	382	MET
1	I	382	MET
1	J	165	THR
1	J	170	GLN
1	J	271	ASN
1	J	382	MET
1	D	270	GLY
1	H	165	THR
1	I	124	SER
1	J	164	CYS
1	C	164	CYS
1	E	164	CYS
1	G	163	GLN
1	H	164	CYS
1	A	124	SER
1	A	164	CYS
1	C	165	THR
1	I	123	GLY
1	J	124	SER
1	E	166	ASN
1	B	125	GLY
1	C	230	PRO
1	B	230	PRO
1	H	169	VAL



### 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	363/432 (84%)	360 (99%)	3 (1%)	81	91
1	B	357/432 (83%)	350 (98%)	7 (2%)	55	78
1	C	363/432 (84%)	359 (99%)	4 (1%)	73	86
1	D	357/432 (83%)	354 (99%)	3 (1%)	81	91
1	E	363/432 (84%)	358 (99%)	5 (1%)	67	83
1	F	355/432 (82%)	353 (99%)	2 (1%)	86	93
1	G	364/432 (84%)	358 (98%)	6 (2%)	62	81
1	H	363/432 (84%)	356 (98%)	7 (2%)	57	79
1	I	354/432 (82%)	351 (99%)	3 (1%)	81	91
1	J	363/432 (84%)	355 (98%)	8 (2%)	52	76
All	All	3602/4320 (83%)	3554 (99%)	48 (1%)	69	84

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	VAL
1	A	267	LYS
1	A	282	ASN
1	B	119	VAL
1	B	121	ASN
1	B	127	ASN
1	B	162	LYS
1	B	229	ASP
1	B	267	LYS
1	B	281	VAL
1	C	119	VAL
1	C	127	ASN
1	C	267	LYS
1	C	281	VAL
1	D	46	ARG
1	D	49	LYS

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Mol	Chain	Res	Type
1	D	282	ASN
1	E	46	ARG
1	E	49	LYS
1	E	119	VAL
1	E	165	THR
1	E	267	LYS
1	F	119	VAL
1	F	267	LYS
1	G	119	VAL
1	G	127	ASN
1	G	170	GLN
1	G	267	LYS
1	G	281	VAL
1	G	432	LEU
1	H	82	ASP
1	H	119	VAL
1	H	170	GLN
1	H	267	LYS
1	H	278	SER
1	H	281	VAL
1	H	282	ASN
1	I	32	SER
1	I	119	VAL
1	I	272	ARG
1	J	119	VAL
1	J	165	THR
1	J	167	THR
1	J	170	GLN
1	J	229	ASP
1	J	281	VAL
1	J	288	LEU
1	J	433	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	130	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	416/496 (83%)	0.03	15 (3%)	42 45	47, 73, 124, 205	0
1	B	410/496 (82%)	0.08	16 (3%)	39 41	56, 87, 150, 194	0
1	C	416/496 (83%)	0.31	30 (7%)	15 18	67, 99, 168, 259	0
1	D	410/496 (82%)	0.19	17 (4%)	37 39	64, 88, 139, 190	0
1	E	416/496 (83%)	0.19	21 (5%)	28 31	70, 93, 152, 222	0
1	F	407/496 (82%)	0.42	26 (6%)	19 21	67, 117, 175, 226	0
1	G	418/496 (84%)	0.36	33 (7%)	12 14	68, 104, 163, 232	0
1	H	416/496 (83%)	0.40	37 (8%)	9 11	62, 103, 161, 236	0
1	I	405/496 (81%)	0.64	47 (11%)	4 5	73, 126, 190, 225	0
1	J	416/496 (83%)	0.43	34 (8%)	11 13	75, 105, 162, 213	0
All	All	4130/4960 (83%)	0.30	276 (6%)	17 20	47, 99, 164, 259	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	426	PRO	12.0
1	H	165	THR	8.8
1	F	392	PHE	8.5
1	C	165	THR	8.2
1	I	392	PHE	7.8
1	E	165	THR	7.1
1	G	392	PHE	7.0
1	F	160	LYS	7.0
1	C	76	PRO	6.7
1	H	166	ASN	6.7
1	G	253	ALA	6.5
1	I	85	THR	6.3
1	J	165	THR	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	77	ASP	6.1
1	I	429	TYR	6.1
1	C	45	LYS	5.9
1	I	35	LEU	5.6
1	I	77	ASP	5.5
1	B	164	CYS	5.4
1	J	429	TYR	5.2
1	B	460	SER	5.2
1	H	392	PHE	5.0
1	G	173	ASP	4.9
1	I	368	SER	4.8
1	I	253	ALA	4.8
1	H	168	PRO	4.6
1	C	164	CYS	4.6
1	D	48	ASN	4.6
1	E	426	PRO	4.6
1	J	392	PHE	4.5
1	I	76	PRO	4.5
1	H	341	SER	4.5
1	D	429	TYR	4.5
1	H	164	CYS	4.4
1	E	166	ASN	4.4
1	H	426	PRO	4.4
1	F	270	GLY	4.4
1	I	88	LEU	4.3
1	A	165	THR	4.2
1	H	342	THR	4.2
1	F	49	LYS	4.2
1	J	170	GLN	4.2
1	B	429	TYR	4.1
1	C	49	LYS	4.1
1	J	124	SER	4.1
1	I	369	ILE	4.0
1	J	50	THR	4.0
1	A	168	PRO	3.9
1	B	392	PHE	3.9
1	G	204	THR	3.9
1	I	314	TRP	3.9
1	F	48	ASN	3.9
1	J	94	GLY	3.8
1	C	335	ALA	3.8
1	J	126	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	426	PRO	3.8
1	H	460	SER	3.8
1	F	369	ILE	3.8
1	J	127	ASN	3.7
1	I	341	SER	3.7
1	G	429	TYR	3.7
1	G	166	ASN	3.7
1	F	426	PRO	3.7
1	C	47	ALA	3.7
1	E	338	THR	3.6
1	E	170	GLN	3.6
1	E	258	GLU	3.6
1	D	368	SER	3.6
1	I	162	LYS	3.6
1	C	127	ASN	3.6
1	G	368	SER	3.6
1	H	70	PRO	3.5
1	J	330	ASN	3.5
1	I	90	TRP	3.5
1	J	387	LEU	3.5
1	H	167	THR	3.5
1	F	370	THR	3.5
1	E	262	ASP	3.5
1	G	165	THR	3.5
1	I	45	LYS	3.4
1	J	176	PRO	3.4
1	I	57	GLY	3.4
1	J	164	CYS	3.3
1	I	367	CYS	3.3
1	C	166	ASN	3.3
1	C	50	THR	3.3
1	E	168	PRO	3.3
1	I	370	THR	3.3
1	H	88	LEU	3.3
1	J	338	THR	3.2
1	H	429	TYR	3.2
1	H	162	LYS	3.2
1	F	77	ASP	3.2
1	G	338	THR	3.2
1	H	441	GLU	3.1
1	F	76	PRO	3.1
1	G	178	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	330	ASN	3.0
1	J	49	LYS	3.0
1	I	428	PRO	3.0
1	C	126	GLY	3.0
1	G	159	GLY	3.0
1	F	85	THR	3.0
1	F	314	TRP	3.0
1	C	427	ASP	3.0
1	I	48	ASN	3.0
1	E	126	GLY	3.0
1	G	268	GLY	3.0
1	A	429	TYR	3.0
1	J	163	GLN	2.9
1	F	47	ALA	2.9
1	I	112	PHE	2.9
1	F	112	PHE	2.9
1	E	79	SER	2.9
1	D	78	SER	2.8
1	D	428	PRO	2.8
1	D	114	ASN	2.8
1	G	426	PRO	2.8
1	D	392	PHE	2.8
1	E	392	PHE	2.8
1	H	118	ASP	2.8
1	B	262	ASP	2.8
1	H	50	THR	2.8
1	A	446	GLU	2.7
1	C	255	GLU	2.7
1	G	254	GLY	2.7
1	A	108	SER	2.7
1	E	460	SER	2.7
1	J	56	SER	2.7
1	H	273	THR	2.7
1	F	269	SER	2.7
1	C	160	LYS	2.7
1	E	76	PRO	2.7
1	E	337	VAL	2.7
1	C	429	TYR	2.7
1	B	445	SER	2.6
1	E	167	THR	2.6
1	F	106	GLY	2.6
1	H	149	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	391	ASN	2.6
1	F	90	TRP	2.6
1	I	56	SER	2.6
1	J	431	ASN	2.6
1	A	329	THR	2.6
1	C	382	MET	2.6
1	F	108	SER	2.6
1	B	195	GLY	2.6
1	G	275	VAL	2.6
1	E	371	LEU	2.6
1	A	77	ASP	2.6
1	D	85	THR	2.6
1	D	106	GLY	2.6
1	G	344	THR	2.6
1	G	339	THR	2.6
1	G	112	PHE	2.5
1	D	338	THR	2.5
1	G	274	SER	2.5
1	E	255	GLU	2.5
1	I	50	THR	2.5
1	J	167	THR	2.5
1	F	382	MET	2.5
1	J	166	ASN	2.5
1	E	164	CYS	2.5
1	H	378	TYR	2.5
1	G	460	SER	2.5
1	H	85	THR	2.5
1	I	254	GLY	2.5
1	A	426	PRO	2.5
1	I	427	ASP	2.5
1	F	390	TRP	2.5
1	G	170	GLN	2.5
1	J	59	GLN	2.5
1	C	328	SER	2.5
1	J	234	ARG	2.5
1	J	443	PHE	2.5
1	A	164	CYS	2.4
1	E	214	CYS	2.4
1	E	50	THR	2.4
1	C	80	LEU	2.4
1	C	330	ASN	2.4
1	D	446	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	426	PRO	2.4
1	I	124	SER	2.4
1	E	77	ASP	2.4
1	B	74	ALA	2.4
1	H	427	ASP	2.4
1	I	379	ILE	2.4
1	C	30	SER	2.4
1	J	192	THR	2.4
1	J	195	GLY	2.4
1	I	149	GLY	2.3
1	D	335	ALA	2.3
1	I	58	TYR	2.3
1	J	329	THR	2.3
1	C	75	LEU	2.3
1	H	340	SER	2.3
1	H	161	GLY	2.3
1	J	391	ASN	2.3
1	G	329	THR	2.3
1	H	126	GLY	2.3
1	F	19	TYR	2.3
1	D	445	SER	2.3
1	I	12	LYS	2.3
1	A	204	THR	2.3
1	I	344	THR	2.3
1	J	135	ASN	2.3
1	I	27	TYR	2.3
1	I	292	GLU	2.3
1	D	330	ASN	2.3
1	G	149	GLY	2.2
1	I	78	SER	2.2
1	B	85	THR	2.2
1	I	204	THR	2.2
1	H	163	GLN	2.2
1	G	78	SER	2.2
1	B	177	LEU	2.2
1	G	269	SER	2.2
1	B	204	THR	2.2
1	J	93	THR	2.2
1	C	161	GLY	2.2
1	H	170	GLN	2.2
1	F	329	THR	2.2
1	H	48	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	147	MET	2.2
1	F	78	SER	2.2
1	G	340	SER	2.2
1	H	127	ASN	2.2
1	J	339	THR	2.2
1	G	382	MET	2.1
1	G	314	TRP	2.1
1	F	89	VAL	2.1
1	B	193	GLY	2.1
1	A	339	THR	2.1
1	F	204	THR	2.1
1	I	234	ARG	2.1
1	J	51	VAL	2.1
1	A	57	GLY	2.1
1	A	102	PRO	2.1
1	C	176	PRO	2.1
1	B	49	LYS	2.1
1	D	262	ASP	2.1
1	G	427	ASP	2.1
1	H	45	LYS	2.1
1	F	338	THR	2.1
1	I	130	GLN	2.1
1	C	102	PRO	2.1
1	G	366	LEU	2.1
1	J	108	SER	2.1
1	H	77	ASP	2.1
1	J	196	ALA	2.1
1	C	338	THR	2.1
1	I	79	SER	2.1
1	H	58	TYR	2.1
1	H	73	PHE	2.1
1	B	12	LYS	2.1
1	I	340	SER	2.1
1	G	303	GLN	2.0
1	H	234	ARG	2.0
1	A	166	ASN	2.0
1	C	48	ASN	2.0
1	H	204	THR	2.0
1	J	40	PRO	2.0
1	I	161	GLY	2.0
1	C	101	GLN	2.0
1	I	374	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	192	THR	2.0
1	H	339	THR	2.0
1	I	342	THR	2.0
1	B	343	TYR	2.0
1	I	47	ALA	2.0
1	I	366	LEU	2.0
1	G	150	CYS	2.0
1	C	336	SER	2.0
1	G	19	TYR	2.0
1	H	79	SER	2.0
1	I	378	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no 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.