



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2026 – 04:35 pm BST

PDB ID : 9RP8 / pdb\_00009rp8  
Title : Crystal structure of the T=1 icosahedral capsid of Turnip Crinkle Virus P38  
Authors : Parthier, C.; Stubbs, M.T.; Golbik, R.P.; Tamilarasan, S.; Behrens, S.-E.  
Deposited on : 2025-06-24  
Resolution : 2.89 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

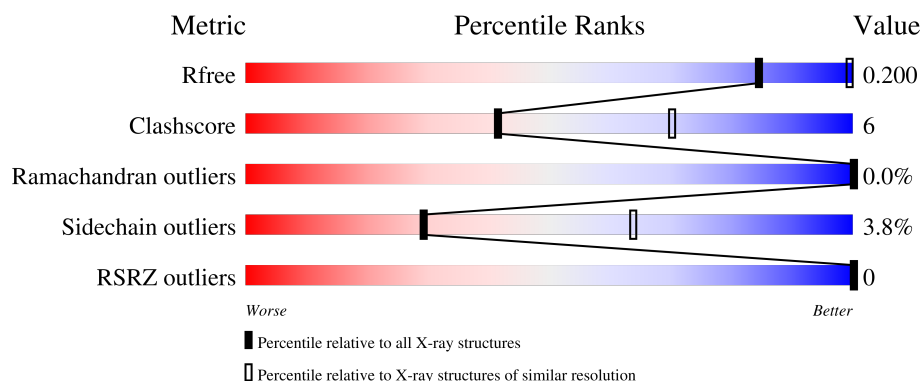
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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  $\geq 3$ , 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	351	
1	B	351	
1	C	351	
1	D	351	
1	E	351	

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Mol	Chain	Length	Quality of chain
1	F	351	
1	G	351	
1	H	351	
1	I	351	
1	J	351	
1	K	351	
1	L	351	
1	M	351	
1	N	351	
1	O	351	
1	P	351	
1	Q	351	
1	R	351	
1	S	351	
1	T	351	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 41357 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	B	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	C	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	D	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	E	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	F	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	G	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	H	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	I	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	J	272	Total	C	N	O	S	0	0	0
			2067	1302	351	409	5			
1	K	272	Total	C	N	O	S	0	0	0
			2067	1302	351	409	5			
1	N	272	Total	C	N	O	S	0	0	0
			2067	1302	351	409	5			
1	M	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	L	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	P	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			
1	O	272	Total	C	N	O	S	0	0	0
			2068	1302	351	410	5			

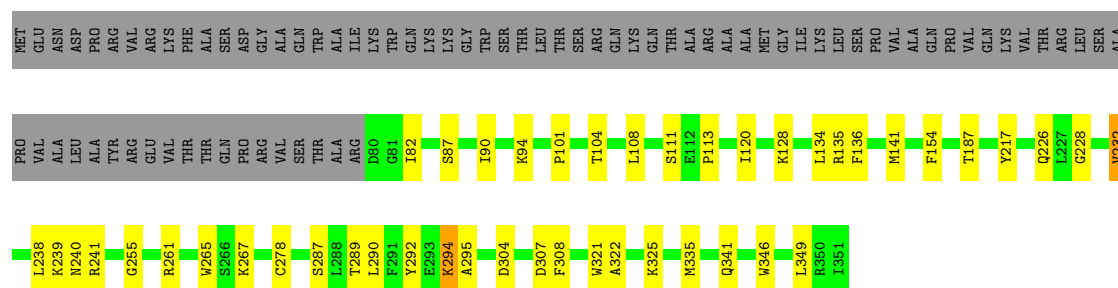
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	272	Total 2068	C 1302	N 351	O 410	S 5	0	0	0
1	S	272	Total 2068	C 1302	N 351	O 410	S 5	0	0	0
1	R	272	Total 2068	C 1302	N 351	O 410	S 5	0	0	0
1	Q	272	Total 2068	C 1302	N 351	O 410	S 5	0	0	0

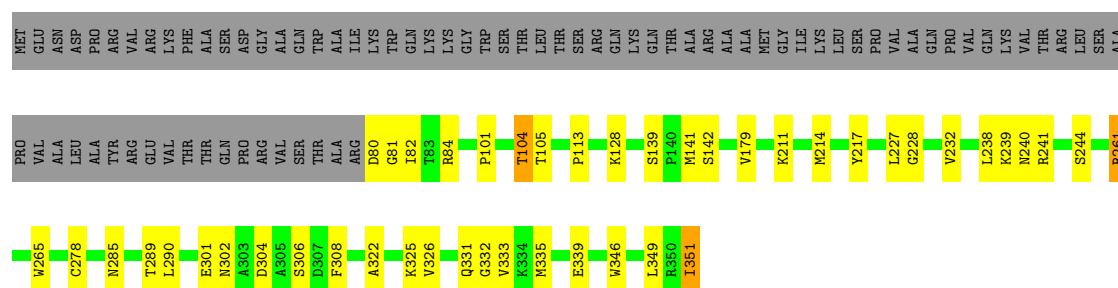


Chain D:  64% 13% 23%



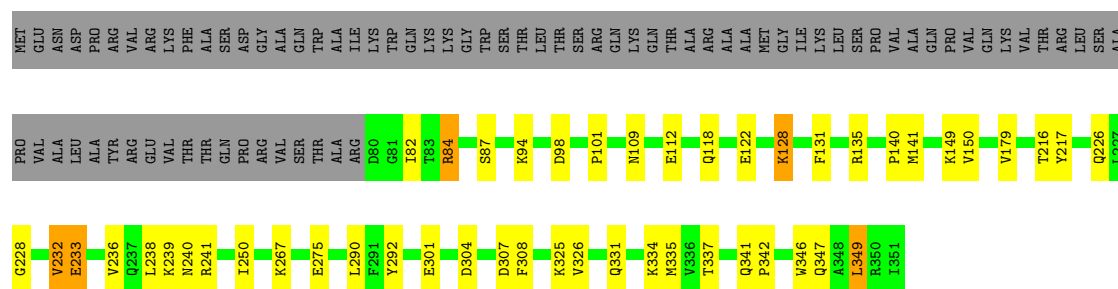
- Molecule 1: Capsid protein

Chain E:  64% 12% 23%



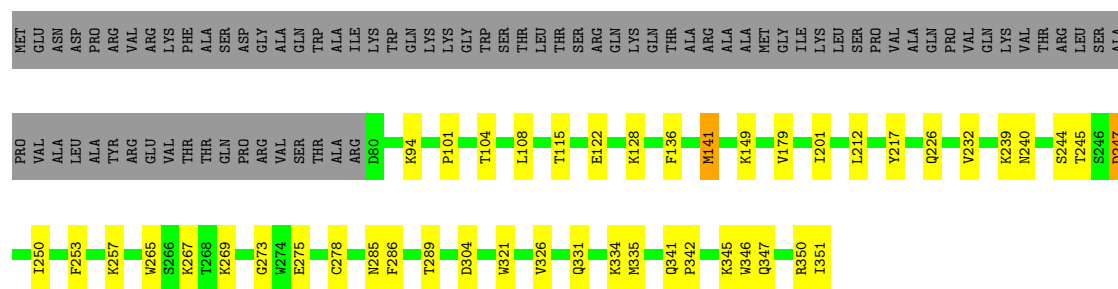
- Molecule 1: Capsid protein

Chain F:  64% 13% 23%



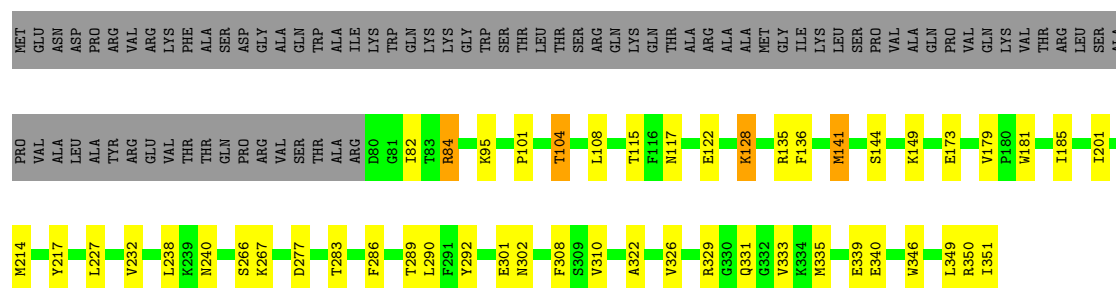
- Molecule 1: Capsid protein

Chain G:  64% 13% 23%



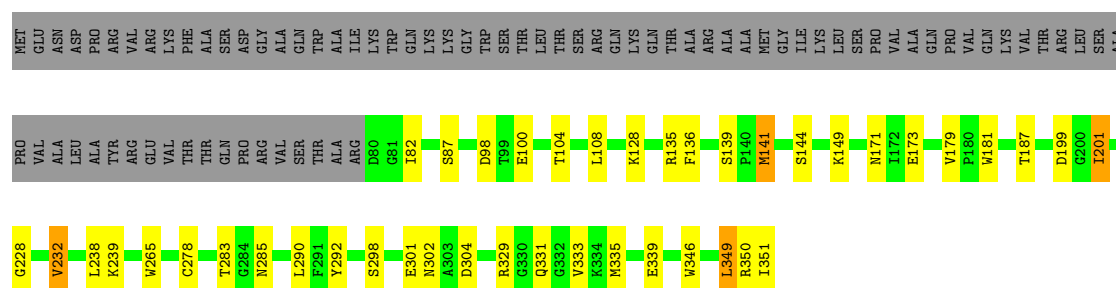
- Molecule 1: Capsid protein

Chain H:  63% 13% 23%



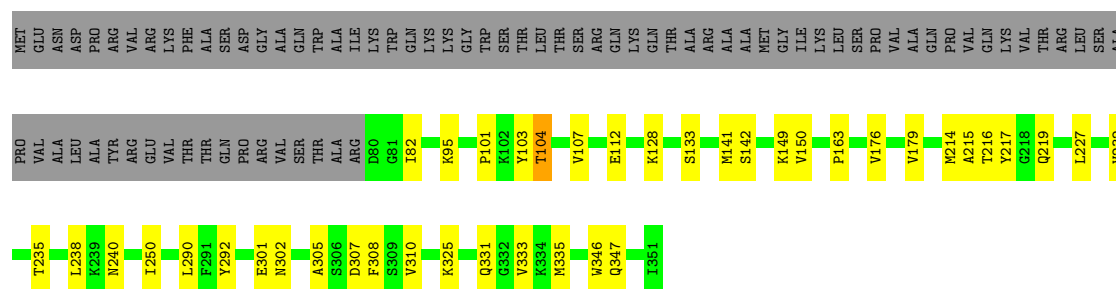
- Molecule 1: Capsid protein

Chain I:  65% 11% 23%



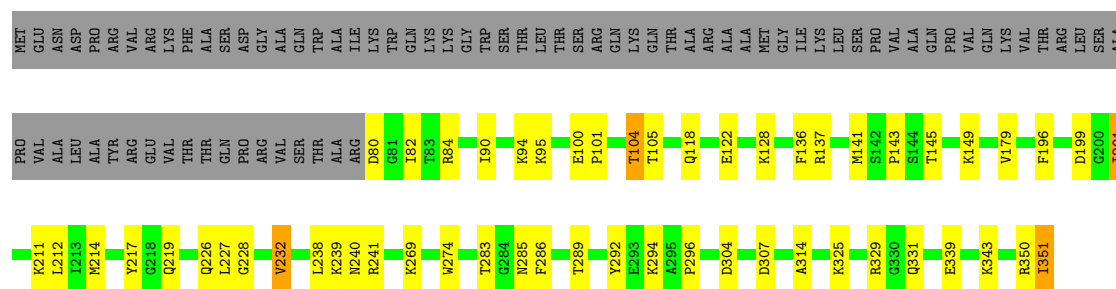
- Molecule 1: Capsid protein

Chain J:  66% 11% 23%



- Molecule 1: Capsid protein

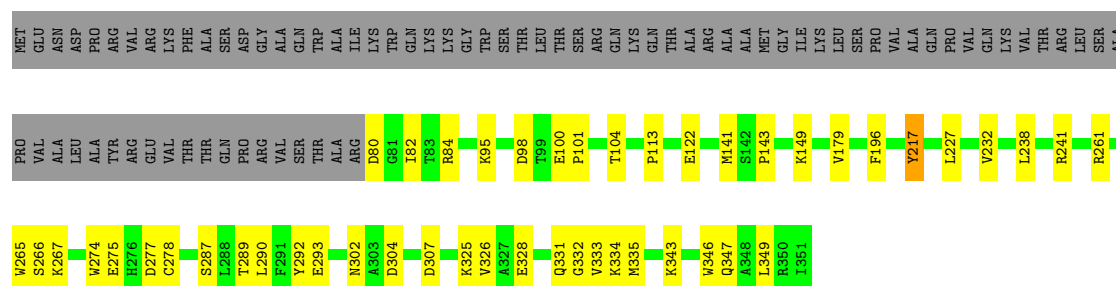
Chain K:  62% 15% 23%



- Molecule 1: Capsid protein

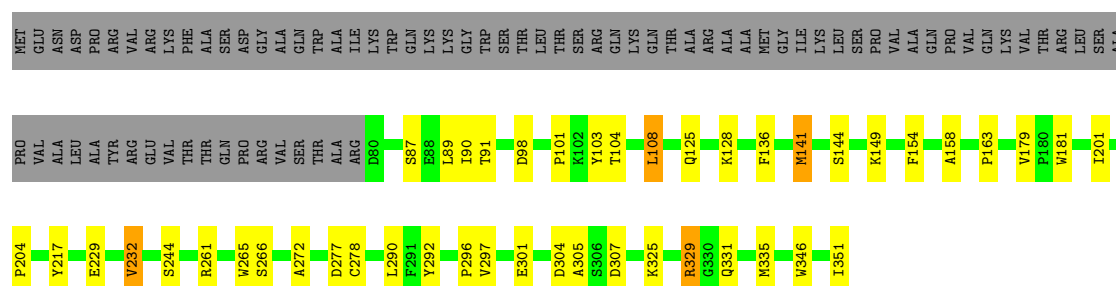


Chain N:  64% 13% 23%



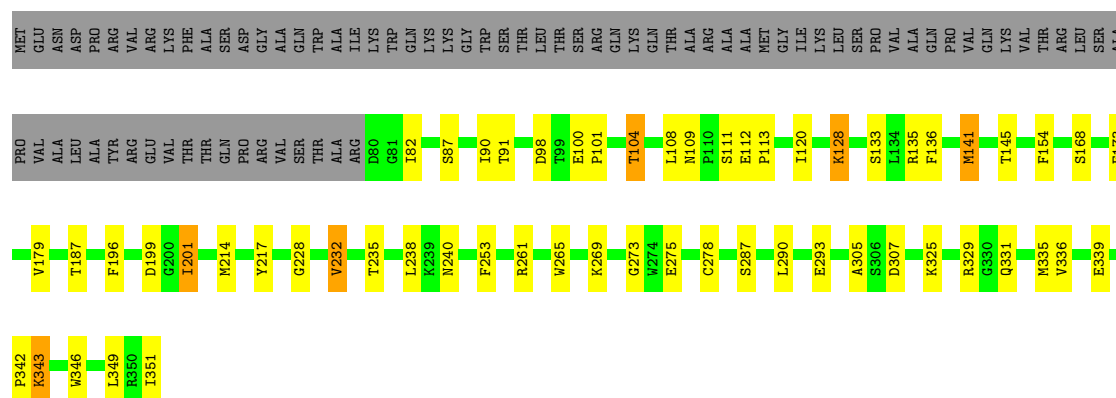
- Molecule 1: Capsid protein

Chain M:  64% 12% 23%



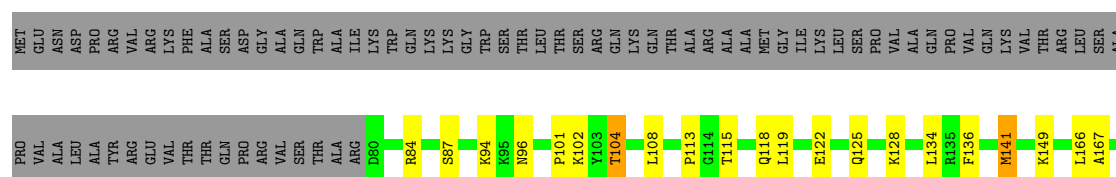
- Molecule 1: Capsid protein

Chain L:  61% 15% 23%



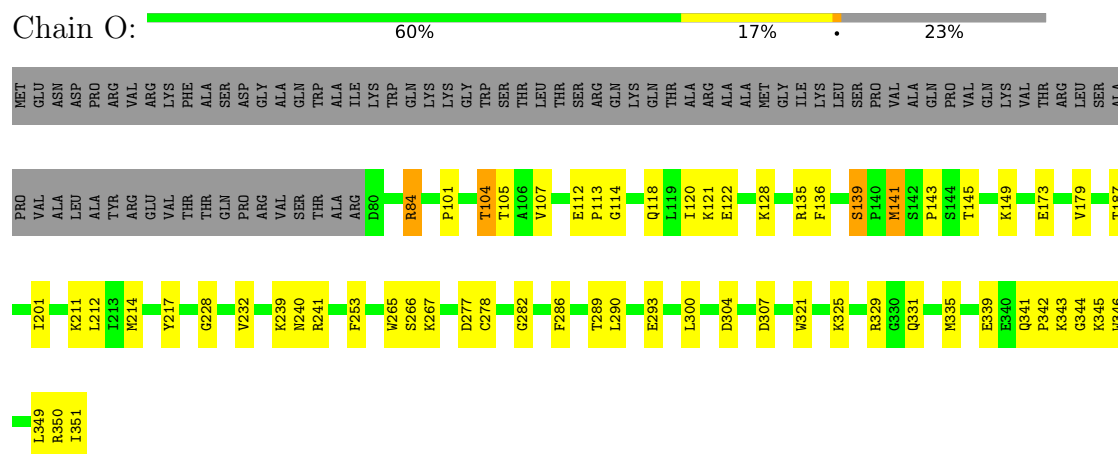
- Molecule 1: Capsid protein

Chain P:  62% 14% 23%

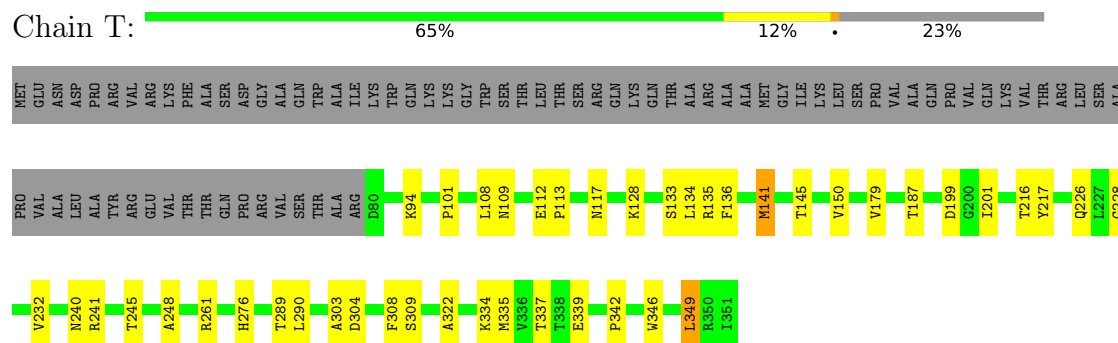




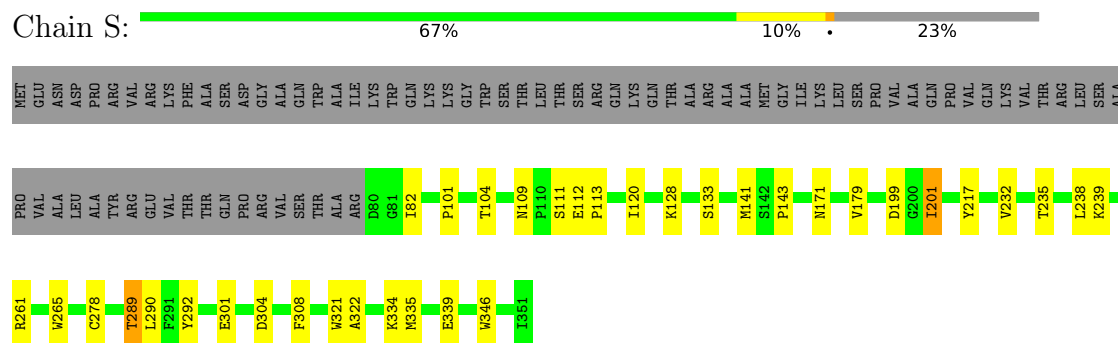
- Molecule 1: Capsid protein



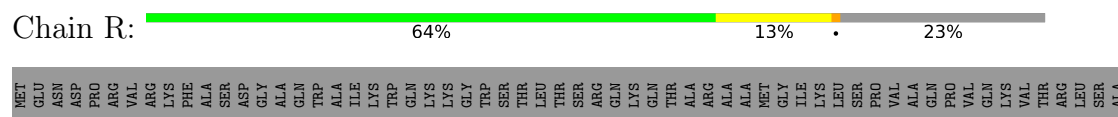
- Molecule 1: Capsid protein

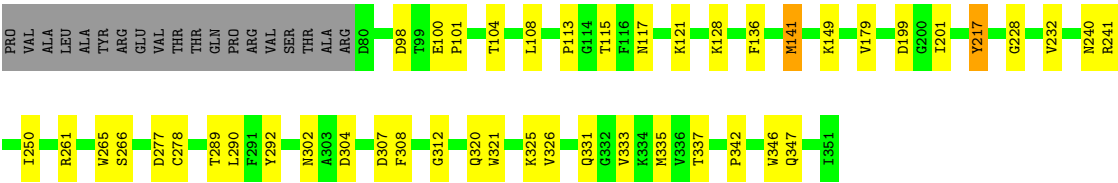


- Molecule 1: Capsid protein

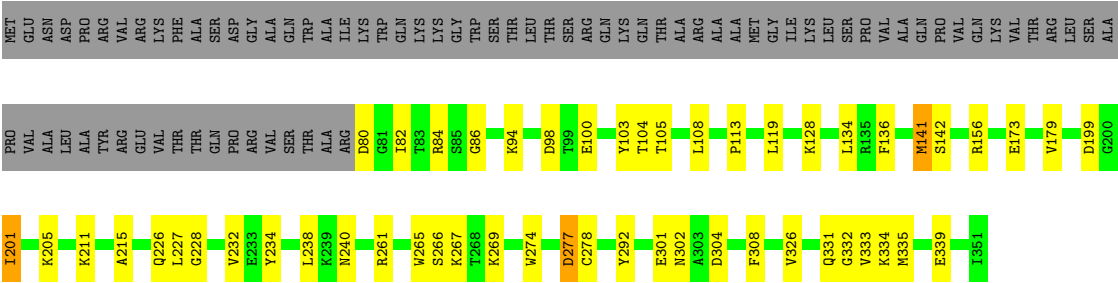
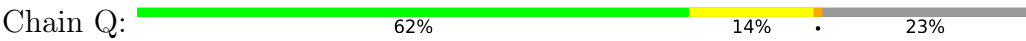


- Molecule 1: Capsid protein





● Molecule 1: Capsid protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.38Å 203.38Å 469.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.81 – 2.89 48.81 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.81-2.89) 99.9 (48.81-2.89)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.173 , 0.193 0.181 , 0.200	Depositor DCC
$R_{free}$ test set	8109 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.339 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.620 for h,-h-k,-l	Depositor
Outliers	0 of 162004 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	41357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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 [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.17	0/2113	0.37	0/2867
1	B	0.18	0/2113	0.39	0/2867
1	C	0.14	0/2113	0.35	0/2867
1	D	0.16	0/2113	0.38	0/2867
1	E	0.17	0/2113	0.37	0/2867
1	F	0.14	0/2113	0.34	0/2867
1	G	0.17	0/2113	0.39	0/2867
1	H	0.16	0/2113	0.37	0/2867
1	I	0.14	0/2113	0.35	0/2867
1	J	0.19	0/2112	0.40	0/2867
1	K	0.15	0/2112	0.35	0/2867
1	L	0.16	0/2113	0.36	0/2867
1	M	0.17	0/2113	0.37	0/2867
1	N	0.16	0/2112	0.37	0/2867
1	O	0.21	0/2113	0.41	0/2867
1	P	0.17	0/2113	0.38	0/2867
1	Q	0.17	0/2113	0.37	0/2867
1	R	0.15	0/2113	0.37	0/2867
1	S	0.18	0/2113	0.35	0/2867
1	T	0.15	0/2113	0.35	0/2867
All	All	0.17	0/42257	0.37	0/57340

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2068	0	2023	25	0
1	B	2068	0	2023	30	0
1	C	2068	0	2023	19	0
1	D	2068	0	2023	26	0
1	E	2068	0	2023	26	0
1	F	2068	0	2023	31	0
1	G	2068	0	2023	30	0
1	H	2068	0	2023	35	0
1	I	2068	0	2023	24	0
1	J	2067	0	2023	26	0
1	K	2067	0	2023	36	0
1	L	2068	0	2023	33	0
1	M	2068	0	2023	29	0
1	N	2067	0	2023	29	0
1	O	2068	0	2023	41	0
1	P	2068	0	2023	33	0
1	Q	2068	0	2023	36	0
1	R	2068	0	2023	29	0
1	S	2068	0	2023	19	0
1	T	2068	0	2023	26	0
All	All	41357	0	40460	526	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 6.

All (526) 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:M:307:ASP:HB2	1:M:325:LYS:HE3	1.31	1.11
1:N:328:GLU:HB2	1:N:331:GLN:HG3	1.40	1.00
1:P:275:GLU:HG2	1:P:336:VAL:HG22	1.55	0.87
1:F:128:LYS:HG3	1:F:240:ASN:HD22	1.39	0.85
1:H:84:ARG:HH21	1:T:241:ARG:HD3	1.43	0.84
1:D:94:LYS:HE2	1:D:226:GLN:HG2	1.64	0.80
1:R:128:LYS:HG3	1:R:240:ASN:HD22	1.45	0.79
1:O:307:ASP:HB3	1:O:325:LYS:HD3	1.65	0.79
1:D:307:ASP:HB3	1:D:325:LYS:HD3	1.65	0.77
1:K:128:LYS:HG3	1:K:240:ASN:HD22	1.50	0.77
1:J:128:LYS:HG3	1:J:240:ASN:HD22	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:290:LEU:HD13	1:O:346:TRP:HB3	1.70	0.73
1:Q:108:LEU:HD11	1:Q:136:PHE:HZ	1.54	0.73
1:G:250:ILE:HD11	1:O:351:ILE:HD11	1.72	0.72
1:T:109:ASN:HB3	1:T:112:GLU:HG2	1.70	0.72
1:T:128:LYS:HG3	1:T:240:ASN:HD22	1.54	0.72
1:E:241:ARG:HD3	1:K:84:ARG:HH21	1.53	0.72
1:B:109:ASN:HB3	1:B:112:GLU:HG2	1.74	0.70
1:L:108:LEU:HD11	1:L:136:PHE:HZ	1.57	0.70
1:J:305:ALA:HA	1:J:331:GLN:HB3	1.75	0.69
1:R:304:ASP:HB2	1:R:331:GLN:HA	1.72	0.69
1:F:307:ASP:HB3	1:F:325:LYS:HD3	1.73	0.69
1:P:241:ARG:HB3	1:O:173:GLU:HG3	1.73	0.69
1:P:326:VAL:HG13	1:P:331:GLN:HB2	1.74	0.69
1:B:173:GLU:HG3	1:F:241:ARG:HB3	1.73	0.69
1:N:349:LEU:HD12	1:P:349:LEU:HD22	1.75	0.69
1:B:82:ILE:HD11	1:B:238:LEU:HD12	1.74	0.69
1:L:109:ASN:HB3	1:L:112:GLU:HG2	1.76	0.68
1:Q:265:TRP:HA	1:Q:277:ASP:O	1.94	0.68
1:D:290:LEU:HD13	1:D:346:TRP:HB3	1.76	0.67
1:B:304:ASP:HB2	1:B:331:GLN:HA	1.74	0.67
1:H:128:LYS:HG3	1:H:240:ASN:HD22	1.58	0.67
1:G:108:LEU:HD11	1:G:136:PHE:HZ	1.59	0.67
1:S:292:TYR:HE2	1:S:335:MET:HE3	1.60	0.67
1:E:290:LEU:HD13	1:E:346:TRP:HB3	1.77	0.66
1:R:108:LEU:HD11	1:R:136:PHE:HZ	1.61	0.66
1:J:301:GLU:HA	1:J:308:PHE:CE2	2.31	0.66
1:J:302:ASN:HA	1:J:333:VAL:HG12	1.76	0.66
1:T:179:VAL:HG12	1:S:141:MET:HA	1.78	0.65
1:T:150:VAL:HG22	1:T:216:THR:HG22	1.79	0.65
1:I:108:LEU:HD11	1:I:136:PHE:HZ	1.62	0.64
1:H:290:LEU:HD13	1:H:346:TRP:HB3	1.78	0.64
1:L:305:ALA:HA	1:L:331:GLN:HB3	1.79	0.64
1:C:82:ILE:HD11	1:C:238:LEU:HD12	1.79	0.63
1:T:135:ARG:HG2	1:T:187:THR:HA	1.80	0.63
1:O:293:GLU:OE2	1:O:343:LYS:HB2	1.99	0.63
1:J:307:ASP:HB2	1:J:325:LYS:HE2	1.81	0.63
1:L:307:ASP:HB2	1:L:325:LYS:HE3	1.79	0.63
1:O:253:PHE:HB2	1:O:342:PRO:O	1.98	0.63
1:T:113:PRO:HG3	1:T:261:ARG:O	1.99	0.63
1:M:290:LEU:HD13	1:M:346:TRP:HB3	1.80	0.63
1:Q:277:ASP:HA	1:Q:334:LYS:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:293:GLU:OE1	1:L:343:LYS:HB2	1.98	0.63
1:J:290:LEU:HD13	1:J:346:TRP:HB3	1.80	0.62
1:C:155:ASP:OD2	1:C:160:LYS:HE2	1.99	0.62
1:N:80:ASP:N	1:Q:173:GLU:OE2	2.33	0.62
1:G:285:ASN:HB3	1:G:351:ILE:HG13	1.82	0.61
1:P:108:LEU:HD11	1:P:136:PHE:HZ	1.65	0.61
1:R:312:GLY:HA3	1:R:320:GLN:HA	1.81	0.61
1:A:108:LEU:HD11	1:A:136:PHE:HZ	1.67	0.60
1:A:292:TYR:HE1	1:A:335:MET:HE3	1.65	0.60
1:N:307:ASP:HB2	1:N:325:LYS:HE2	1.83	0.60
1:G:128:LYS:HB2	1:G:239:LYS:HG3	1.83	0.60
1:J:128:LYS:HG3	1:J:240:ASN:ND2	2.17	0.60
1:O:304:ASP:OD2	1:O:331:GLN:HA	2.01	0.60
1:N:304:ASP:HB2	1:N:331:GLN:HA	1.81	0.60
1:F:82:ILE:HD11	1:F:238:LEU:HD12	1.82	0.60
1:P:128:LYS:HG3	1:P:240:ASN:HD22	1.66	0.60
1:S:109:ASN:HB3	1:S:112:GLU:HG2	1.84	0.60
1:S:113:PRO:HG3	1:S:261:ARG:O	2.02	0.59
1:F:109:ASN:HB3	1:F:112:GLU:HG2	1.83	0.59
1:B:285:ASN:HB3	1:B:351:ILE:HG23	1.85	0.59
1:M:101:PRO:HA	1:M:217:TYR:HB3	1.84	0.59
1:I:173:GLU:HG3	1:T:241:ARG:HB3	1.84	0.59
1:A:272:ALA:HB1	1:A:297:VAL:HG11	1.85	0.58
1:D:128:LYS:HB2	1:D:239:LYS:HG3	1.85	0.58
1:H:82:ILE:HD11	1:H:238:LEU:HD12	1.84	0.58
1:T:108:LEU:HD11	1:T:136:PHE:HZ	1.68	0.58
1:J:250:ILE:HG12	1:J:347:GLN:HG3	1.85	0.58
1:I:98:ASP:OD2	1:I:100:GLU:HB2	2.03	0.58
1:G:275:GLU:OE2	1:G:334:LYS:HD2	2.02	0.58
1:P:119:LEU:HB2	1:P:234:TYR:OH	2.03	0.58
1:B:290:LEU:HD13	1:B:346:TRP:HB3	1.86	0.58
1:S:101:PRO:HA	1:S:217:TYR:HB3	1.86	0.58
1:I:290:LEU:HD13	1:I:346:TRP:HB3	1.84	0.58
1:F:150:VAL:HG22	1:F:216:THR:HG22	1.86	0.57
1:D:108:LEU:HD11	1:D:136:PHE:HZ	1.69	0.57
1:G:128:LYS:HG3	1:G:240:ASN:OD1	2.03	0.57
1:D:135:ARG:HG2	1:D:187:THR:HA	1.86	0.57
1:N:101:PRO:HA	1:N:217:TYR:HB3	1.85	0.57
1:R:113:PRO:HG3	1:R:261:ARG:O	2.04	0.57
1:Q:94:LYS:HE2	1:Q:226:GLN:HG2	1.87	0.57
1:Q:302:ASN:HA	1:Q:333:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:PHE:HB2	1:B:342:PRO:O	2.05	0.57
1:K:304:ASP:OD2	1:K:331:GLN:HA	2.04	0.57
1:M:108:LEU:HD21	1:M:136:PHE:HZ	1.69	0.56
1:F:337:THR:HG21	1:F:342:PRO:HG3	1.86	0.56
1:H:173:GLU:HG3	1:O:241:ARG:NH2	2.20	0.56
1:J:307:ASP:HB3	1:J:325:LYS:HB3	1.87	0.56
1:R:149:LYS:HG3	1:Q:141:MET:HE3	1.87	0.56
1:F:101:PRO:HA	1:F:217:TYR:HB3	1.87	0.56
1:A:101:PRO:HA	1:A:217:TYR:HB3	1.88	0.56
1:A:290:LEU:HD13	1:A:346:TRP:HB3	1.86	0.56
1:B:282:GLY:HA2	1:B:329:ARG:HD3	1.88	0.56
1:E:241:ARG:HB3	1:L:173:GLU:HG3	1.88	0.56
1:D:292:TYR:HE1	1:D:335:MET:HE3	1.71	0.56
1:T:290:LEU:HD13	1:T:346:TRP:HB3	1.87	0.55
1:S:82:ILE:HD11	1:S:238:LEU:HD12	1.88	0.55
1:S:290:LEU:HD13	1:S:346:TRP:HB3	1.86	0.55
1:B:141:MET:HE3	1:C:149:LYS:HG3	1.88	0.55
1:I:283:THR:HG23	1:I:329:ARG:HG3	1.88	0.55
1:N:275:GLU:OE2	1:N:334:LYS:HD2	2.07	0.55
1:A:128:LYS:HB2	1:A:239:LYS:HG3	1.89	0.55
1:M:304:ASP:OD2	1:M:331:GLN:HA	2.06	0.55
1:H:301:GLU:HA	1:H:308:PHE:CE2	2.42	0.55
1:P:149:LYS:HB3	1:P:217:TYR:CE1	2.42	0.55
1:E:289:THR:HG21	1:K:289:THR:HG21	1.87	0.55
1:K:101:PRO:HA	1:K:217:TYR:HB3	1.89	0.55
1:L:135:ARG:HG2	1:L:187:THR:HA	1.88	0.55
1:O:113:PRO:HA	1:O:120:ILE:HD12	1.89	0.55
1:Q:84:ARG:NH1	1:Q:234:TYR:CZ	2.74	0.55
1:K:149:LYS:HG3	1:O:141:MET:HE3	1.87	0.55
1:S:301:GLU:OE2	1:S:334:LYS:HE3	2.07	0.55
1:F:290:LEU:HD13	1:F:346:TRP:HB3	1.89	0.55
1:H:289:THR:HG21	1:T:289:THR:HG21	1.89	0.55
1:O:135:ARG:HG2	1:O:187:THR:HA	1.88	0.55
1:E:304:ASP:OD2	1:E:331:GLN:HA	2.07	0.55
1:G:326:VAL:HG13	1:G:331:GLN:HB2	1.89	0.54
1:B:283:THR:HG23	1:B:329:ARG:HG3	1.88	0.54
1:H:108:LEU:HD11	1:H:136:PHE:HZ	1.73	0.54
1:F:275:GLU:OE2	1:F:334:LYS:HD2	2.07	0.54
1:M:91:THR:HB	1:M:329:ARG:HH21	1.72	0.54
1:B:173:GLU:CD	1:F:241:ARG:H	2.15	0.54
1:P:113:PRO:HG3	1:P:261:ARG:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:ARG:NH2	1:T:241:ARG:HD3	2.17	0.54
1:K:128:LYS:HG3	1:K:240:ASN:ND2	2.21	0.54
1:N:267:LYS:HD3	1:N:274:TRP:CZ3	2.43	0.54
1:I:82:ILE:HD11	1:I:238:LEU:HD12	1.89	0.54
1:B:248:ALA:HB2	1:B:349:LEU:HD12	1.90	0.54
1:D:287:SER:HB3	1:D:349:LEU:HD11	1.90	0.54
1:P:292:TYR:HE2	1:P:335:MET:HE3	1.73	0.53
1:Q:82:ILE:HD11	1:Q:238:LEU:HD12	1.91	0.53
1:H:349:LEU:HD22	1:T:349:LEU:HD22	1.91	0.53
1:P:141:MET:HG2	1:P:228:GLY:HA2	1.91	0.53
1:T:337:THR:HG21	1:T:342:PRO:HG3	1.90	0.53
1:R:302:ASN:HA	1:R:333:VAL:HG12	1.90	0.53
1:B:292:TYR:HE1	1:B:335:MET:HE3	1.74	0.53
1:K:104:THR:HB	1:K:214:MET:HE3	1.91	0.53
1:L:293:GLU:CD	1:L:343:LYS:HB2	2.34	0.53
1:D:113:PRO:HG3	1:D:261:ARG:O	2.09	0.53
1:G:269:LYS:HG2	1:G:273:GLY:O	2.08	0.53
1:I:141:MET:HE3	1:J:149:LYS:HG3	1.90	0.52
1:Q:304:ASP:OD2	1:Q:331:GLN:HA	2.10	0.52
1:B:113:PRO:HG3	1:B:261:ARG:O	2.10	0.52
1:I:135:ARG:HG2	1:I:187:THR:HA	1.90	0.52
1:M:265:TRP:CH2	1:M:278:CYS:HB2	2.45	0.52
1:F:131:PHE:CD1	1:F:236:VAL:HB	2.44	0.52
1:E:141:MET:HG2	1:E:228:GLY:HA2	1.90	0.52
1:L:82:ILE:HD11	1:L:238:LEU:HD12	1.91	0.52
1:L:111:SER:HA	1:L:120:ILE:HG13	1.92	0.52
1:H:302:ASN:HA	1:H:333:VAL:HG12	1.91	0.52
1:L:199:ASP:OD2	1:L:201:ILE:HD11	2.09	0.52
1:K:95:LYS:HB2	1:K:219:GLN:HG2	1.91	0.52
1:N:84:ARG:NH2	1:P:241:ARG:HD3	2.25	0.52
1:R:108:LEU:HD23	1:R:115:THR:HG21	1.92	0.52
1:E:302:ASN:HA	1:E:333:VAL:HG12	1.91	0.51
1:J:95:LYS:HB2	1:J:219:GLN:HG2	1.91	0.51
1:L:275:GLU:HG2	1:L:336:VAL:HG22	1.91	0.51
1:P:104:THR:HB	1:P:214:MET:HE3	1.91	0.51
1:N:290:LEU:HD13	1:N:346:TRP:HB3	1.90	0.51
1:M:158:ALA:HB3	1:M:204:PRO:HB3	1.92	0.51
1:L:307:ASP:HB3	1:L:325:LYS:HB3	1.93	0.51
1:O:128:LYS:HB2	1:O:239:LYS:HG3	1.92	0.51
1:E:308:PHE:HE1	1:E:322:ALA:HB1	1.76	0.51
1:G:101:PRO:HA	1:G:217:TYR:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:337:THR:HG21	1:R:342:PRO:HG3	1.93	0.51
1:F:292:TYR:HE2	1:F:335:MET:HE3	1.76	0.51
1:S:128:LYS:HB2	1:S:239:LYS:HG3	1.93	0.51
1:J:142:SER:OG	1:J:227:LEU:HA	2.11	0.51
1:L:113:PRO:HG3	1:L:261:ARG:O	2.11	0.51
1:R:290:LEU:HD13	1:R:346:TRP:HB3	1.93	0.51
1:Q:119:LEU:HD22	1:Q:234:TYR:CE2	2.46	0.51
1:G:345:LYS:HE3	1:O:321:TRP:CH2	2.46	0.51
1:F:94:LYS:HE2	1:F:226:GLN:HG2	1.93	0.50
1:S:265:TRP:CH2	1:S:278:CYS:HB2	2.46	0.50
1:O:84:ARG:HD2	1:O:122:GLU:OE2	2.12	0.50
1:Q:98:ASP:OD2	1:Q:100:GLU:HB2	2.11	0.50
1:C:141:MET:HG2	1:C:228:GLY:HA2	1.93	0.50
1:E:82:ILE:HD11	1:E:238:LEU:HD12	1.93	0.50
1:F:128:LYS:HG3	1:F:240:ASN:ND2	2.18	0.50
1:H:308:PHE:HE1	1:H:322:ALA:HB1	1.77	0.50
1:G:253:PHE:HB2	1:G:342:PRO:O	2.11	0.50
1:B:307:ASP:HB3	1:B:325:LYS:HB2	1.92	0.50
1:K:105:THR:HB	1:K:211:LYS:HD2	1.93	0.50
1:O:107:VAL:O	1:O:112:GLU:HG3	2.12	0.50
1:S:171:ASN:HD21	1:R:117:ASN:ND2	2.09	0.50
1:D:108:LEU:HD12	1:D:154:PHE:CE2	2.46	0.50
1:I:349:LEU:HG	1:I:350:ARG:N	2.26	0.50
1:F:84:ARG:HH12	1:F:118:GLN:HB3	1.77	0.50
1:H:84:ARG:HH11	1:H:122:GLU:HG3	1.77	0.50
1:H:141:MET:HE3	1:I:149:LYS:HG3	1.94	0.50
1:K:90:ILE:HD11	1:K:232:VAL:HB	1.93	0.49
1:L:290:LEU:HD13	1:L:346:TRP:HB3	1.94	0.49
1:Q:199:ASP:OD2	1:Q:201:ILE:HD11	2.12	0.49
1:C:290:LEU:HD13	1:C:346:TRP:HB3	1.93	0.49
1:P:101:PRO:HA	1:P:217:TYR:HB3	1.94	0.49
1:L:128:LYS:HG3	1:L:240:ASN:HD22	1.76	0.49
1:M:305:ALA:HA	1:M:331:GLN:HB3	1.94	0.49
1:O:253:PHE:HD1	1:O:344:GLY:H	1.60	0.49
1:S:171:ASN:HD21	1:R:117:ASN:HD21	1.59	0.49
1:G:286:PHE:CE2	1:G:350:ARG:HG2	2.48	0.49
1:N:326:VAL:HG13	1:N:331:GLN:HB2	1.94	0.49
1:T:303:ALA:HB2	1:T:334:LYS:HG3	1.93	0.49
1:K:82:ILE:HD11	1:K:238:LEU:HD12	1.94	0.49
1:K:199:ASP:OD2	1:K:201:ILE:HD11	2.12	0.49
1:K:292:TYR:CE2	1:K:296:PRO:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:NH2	1:F:241:ARG:HD3	2.27	0.49
1:G:108:LEU:HD23	1:G:115:THR:HG21	1.94	0.49
1:G:304:ASP:OD2	1:G:331:GLN:HA	2.13	0.49
1:D:82:ILE:HD11	1:D:238:LEU:HD12	1.94	0.49
1:H:117:ASN:ND2	1:I:171:ASN:HD21	2.11	0.49
1:J:150:VAL:HG22	1:J:216:THR:HG22	1.95	0.49
1:L:287:SER:HB3	1:L:349:LEU:HD11	1.94	0.48
1:O:267:LYS:NZ	1:O:341:GLN:HG2	2.28	0.48
1:R:250:ILE:HG12	1:R:347:GLN:HG3	1.94	0.48
1:H:301:GLU:HA	1:H:308:PHE:HE2	1.78	0.48
1:K:307:ASP:HB2	1:K:325:LYS:HE2	1.96	0.48
1:H:292:TYR:HE1	1:H:335:MET:HE3	1.78	0.48
1:Q:84:ARG:NH1	1:Q:86:GLY:HA3	2.29	0.48
1:G:257:LYS:HG2	1:G:346:TRP:HZ2	1.78	0.48
1:N:82:ILE:HD11	1:N:238:LEU:HD12	1.94	0.48
1:F:267:LYS:NZ	1:F:341:GLN:HG2	2.29	0.48
1:M:90:ILE:HG22	1:M:329:ARG:NH2	2.28	0.48
1:T:141:MET:HG2	1:T:228:GLY:HA2	1.95	0.48
1:G:141:MET:HE3	1:H:149:LYS:HG3	1.95	0.48
1:K:136:PHE:CD2	1:K:212:LEU:HD22	2.48	0.48
1:L:91:THR:HB	1:L:329:ARG:HH22	1.78	0.48
1:D:265:TRP:CH2	1:D:278:CYS:HB2	2.48	0.48
1:K:283:THR:HG23	1:K:329:ARG:HG3	1.94	0.48
1:R:199:ASP:OD2	1:R:201:ILE:HG12	2.14	0.48
1:E:128:LYS:HB2	1:E:239:LYS:HG3	1.94	0.48
1:I:141:MET:HG2	1:I:228:GLY:HA2	1.96	0.48
1:N:143:PRO:HB3	1:O:145:THR:O	2.14	0.48
1:A:90:ILE:HD11	1:A:232:VAL:HB	1.95	0.47
1:E:326:VAL:HG13	1:E:331:GLN:HB2	1.96	0.47
1:J:292:TYR:HE1	1:J:335:MET:HE3	1.79	0.47
1:O:286:PHE:HA	1:O:351:ILE:H	1.79	0.47
1:G:265:TRP:CH2	1:G:278:CYS:HB2	2.49	0.47
1:H:308:PHE:CZ	1:H:310:VAL:HB	2.49	0.47
1:K:84:ARG:HD2	1:K:122:GLU:OE2	2.14	0.47
1:K:201:ILE:H	1:K:201:ILE:HG13	1.60	0.47
1:R:292:TYR:HE1	1:R:335:MET:HE3	1.80	0.47
1:J:308:PHE:CZ	1:J:310:VAL:HB	2.49	0.47
1:L:98:ASP:OD2	1:L:100:GLU:HB2	2.14	0.47
1:P:108:LEU:HD23	1:P:115:THR:HG21	1.95	0.47
1:E:101:PRO:HA	1:E:217:TYR:HB3	1.96	0.47
1:F:141:MET:HG2	1:F:228:GLY:HA2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:298:SER:OG	1:I:301:GLU:OE2	2.31	0.47
1:P:84:ARG:HD2	1:P:122:GLU:OE1	2.14	0.47
1:D:90:ILE:HD11	1:D:232:VAL:HB	1.96	0.47
1:D:108:LEU:HD23	1:D:108:LEU:HA	1.65	0.47
1:E:142:SER:OG	1:E:227:LEU:HA	2.15	0.47
1:I:304:ASP:OD2	1:I:331:GLN:HA	2.14	0.47
1:J:107:VAL:O	1:J:112:GLU:HG3	2.14	0.47
1:P:96:ASN:CG	1:P:102:LYS:HE2	2.40	0.47
1:Q:142:SER:OG	1:Q:227:LEU:HA	2.14	0.47
1:D:141:MET:HG2	1:D:228:GLY:HA2	1.97	0.47
1:E:128:LYS:HG3	1:E:240:ASN:OD1	2.14	0.47
1:E:285:ASN:HB3	1:E:351:ILE:HG13	1.97	0.47
1:H:128:LYS:HG3	1:H:240:ASN:ND2	2.27	0.47
1:Q:266:SER:HB3	1:Q:277:ASP:HB2	1.97	0.47
1:L:253:PHE:HB2	1:L:342:PRO:O	2.14	0.47
1:O:104:THR:HB	1:O:214:MET:HE3	1.97	0.47
1:Q:266:SER:HB3	1:Q:277:ASP:CG	2.40	0.47
1:H:326:VAL:HG13	1:H:331:GLN:HB2	1.97	0.47
1:J:307:ASP:CB	1:J:325:LYS:HB3	2.45	0.47
1:K:286:PHE:CE2	1:K:350:ARG:HG2	2.50	0.47
1:E:113:PRO:HG3	1:E:261:ARG:O	2.15	0.46
1:M:90:ILE:HD11	1:M:232:VAL:HB	1.97	0.46
1:C:293:GLU:HB2	1:C:343:LYS:O	2.16	0.46
1:N:287:SER:HB3	1:N:349:LEU:HD22	1.97	0.46
1:N:293:GLU:HB2	1:N:343:LYS:O	2.15	0.46
1:C:108:LEU:HD11	1:C:136:PHE:HZ	1.80	0.46
1:D:108:LEU:HD12	1:D:154:PHE:HE2	1.78	0.46
1:J:101:PRO:HA	1:J:217:TYR:HB3	1.97	0.46
1:L:90:ILE:HD11	1:L:232:VAL:HB	1.95	0.46
1:C:113:PRO:HG3	1:C:261:ARG:O	2.15	0.46
1:K:141:MET:HG2	1:K:228:GLY:HA2	1.96	0.46
1:P:167:ALA:HB1	1:T:117:ASN:ND2	2.30	0.46
1:I:285:ASN:HB3	1:I:351:ILE:HG13	1.98	0.46
1:L:101:PRO:HA	1:L:217:TYR:HB3	1.98	0.46
1:T:94:LYS:HE2	1:T:226:GLN:HG2	1.96	0.46
1:Q:108:LEU:HD23	1:Q:108:LEU:HA	1.75	0.46
1:B:95:LYS:HA	1:B:227:LEU:HD11	1.97	0.46
1:B:308:PHE:CZ	1:B:310:VAL:HB	2.51	0.46
1:G:247:ASP:OD1	1:O:121:LYS:HE3	2.16	0.46
1:H:286:PHE:CE2	1:H:350:ARG:HG2	2.50	0.46
1:N:95:LYS:HA	1:N:227:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:101:PRO:HA	1:O:217:TYR:HB3	1.96	0.46
1:Q:103:TYR:CE1	1:Q:215:ALA:HB2	2.51	0.46
1:R:199:ASP:CG	1:R:201:ILE:HG12	2.41	0.46
1:M:89:LEU:HD11	1:M:229:GLU:HB3	1.97	0.46
1:E:104:THR:HB	1:E:214:MET:HE3	1.97	0.46
1:M:307:ASP:CB	1:M:325:LYS:HE3	2.23	0.46
1:S:111:SER:HA	1:S:120:ILE:HG13	1.97	0.46
1:C:136:PHE:CD2	1:C:212:LEU:HD13	2.50	0.46
1:E:84:ARG:NH2	1:K:241:ARG:HD3	2.31	0.46
1:J:335:MET:HE2	1:J:335:MET:HB2	1.89	0.46
1:L:265:TRP:CH2	1:L:278:CYS:HB2	2.51	0.46
1:P:265:TRP:CH2	1:P:278:CYS:HB2	2.51	0.46
1:F:304:ASP:HB2	1:F:331:GLN:HA	1.97	0.45
1:M:91:THR:HB	1:M:329:ARG:NH2	2.31	0.45
1:P:84:ARG:HH22	1:P:118:GLN:HB3	1.80	0.45
1:C:101:PRO:HA	1:C:217:TYR:HB3	1.98	0.45
1:I:139:SER:HB3	1:J:149:LYS:HZ1	1.80	0.45
1:P:87:SER:HB2	1:P:233:GLU:HG2	1.97	0.45
1:S:301:GLU:HA	1:S:308:PHE:HE2	1.81	0.45
1:Q:265:TRP:CH2	1:Q:278:CYS:HB2	2.51	0.45
1:F:326:VAL:HG13	1:F:331:GLN:HB2	1.97	0.45
1:M:272:ALA:HB1	1:M:297:VAL:HG11	1.96	0.45
1:O:141:MET:HG2	1:O:228:GLY:HA2	1.97	0.45
1:J:95:LYS:HA	1:J:227:LEU:HD11	1.97	0.45
1:J:133:SER:HB3	1:J:235:THR:HB	1.97	0.45
1:T:108:LEU:CD1	1:T:134:LEU:HD21	2.46	0.45
1:E:335:MET:HE2	1:E:335:MET:HB2	1.86	0.45
1:F:135:ARG:HB2	1:F:233:GLU:HG3	1.98	0.45
1:F:250:ILE:HG13	1:F:347:GLN:HG3	1.98	0.45
1:Q:108:LEU:CD1	1:Q:134:LEU:HD21	2.47	0.45
1:B:267:LYS:HG2	1:B:274:TRP:CE3	2.52	0.45
1:D:308:PHE:HE1	1:D:322:ALA:HB1	1.82	0.45
1:G:321:TRP:CH2	1:O:345:LYS:HE3	2.52	0.45
1:H:104:THR:HB	1:H:214:MET:HE3	1.98	0.45
1:M:108:LEU:HD23	1:M:154:PHE:CE1	2.51	0.45
1:Q:269:LYS:HD3	1:Q:274:TRP:CZ2	2.52	0.45
1:C:199:ASP:OD2	1:C:201:ILE:HG12	2.16	0.45
1:A:136:PHE:CD1	1:A:212:LEU:HD22	2.52	0.45
1:E:244:SER:HB3	1:K:118:GLN:HE21	1.82	0.45
1:H:267:LYS:HD3	1:H:340:GLU:HG3	1.98	0.45
1:Q:301:GLU:HA	1:Q:308:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LYS:NZ	1:D:341:GLN:HG2	2.32	0.44
1:G:335:MET:HE2	1:G:335:MET:HB2	1.84	0.44
1:L:269:LYS:HG2	1:L:273:GLY:O	2.16	0.44
1:D:128:LYS:HG3	1:D:240:ASN:OD1	2.17	0.44
1:G:94:LYS:HE2	1:G:226:GLN:HG2	1.98	0.44
1:R:266:SER:OG	1:R:277:ASP:HB2	2.17	0.44
1:Q:113:PRO:HG3	1:Q:261:ARG:O	2.16	0.44
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.70	0.44
1:H:101:PRO:HA	1:H:217:TYR:HB3	1.99	0.44
1:H:351:ILE:CD1	1:T:248:ALA:HB3	2.47	0.44
1:K:294:LYS:HE3	1:K:343:LYS:NZ	2.33	0.44
1:N:98:ASP:OD2	1:N:100:GLU:HB2	2.17	0.44
1:N:335:MET:HE2	1:N:335:MET:HB2	1.90	0.44
1:Q:326:VAL:HG13	1:Q:331:GLN:HB2	1.98	0.44
1:A:87:SER:HA	1:A:232:VAL:O	2.17	0.44
1:M:307:ASP:N	1:M:325:LYS:HB3	2.32	0.44
1:P:125:GLN:HG2	1:P:244:SER:HB3	2.00	0.44
1:G:244:SER:OG	1:O:118:GLN:HG2	2.17	0.44
1:Q:278:CYS:O	1:Q:332:GLY:HA3	2.17	0.44
1:B:301:GLU:HA	1:B:308:PHE:CE2	2.52	0.44
1:I:199:ASP:OD2	1:I:201:ILE:HD11	2.17	0.44
1:M:149:LYS:HG3	1:L:141:MET:HE3	2.00	0.44
1:R:289:THR:HG22	1:R:321:TRP:CD1	2.53	0.44
1:Q:119:LEU:HB2	1:Q:234:TYR:OH	2.17	0.44
1:Q:277:ASP:N	1:Q:277:ASP:OD1	2.51	0.44
1:A:108:LEU:CD1	1:A:134:LEU:HD21	2.48	0.44
1:K:145:THR:O	1:O:143:PRO:HB3	2.18	0.44
1:M:144:SER:HA	1:M:181:TRP:CG	2.53	0.44
1:T:308:PHE:HE1	1:T:322:ALA:HB1	1.83	0.44
1:B:95:LYS:HB2	1:B:219:GLN:HG2	1.99	0.44
1:D:111:SER:HA	1:D:120:ILE:HG13	2.00	0.44
1:F:140:PRO:O	1:G:149:LYS:HE2	2.17	0.44
1:G:122:GLU:OE2	1:O:122:GLU:CD	2.61	0.44
1:N:265:TRP:CH2	1:N:278:CYS:HB2	2.52	0.44
1:P:290:LEU:HD13	1:P:346:TRP:HB3	2.00	0.44
1:Q:128:LYS:HG3	1:Q:240:ASN:OD1	2.18	0.44
1:G:289:THR:OG1	1:G:347:GLN:HB3	2.17	0.44
1:R:265:TRP:CH2	1:R:278:CYS:HB2	2.53	0.44
1:B:325:LYS:HD3	1:B:325:LYS:N	2.33	0.43
1:I:265:TRP:CH2	1:I:278:CYS:HB2	2.52	0.43
1:I:87:SER:HA	1:I:232:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:SER:HA	1:H:181:TRP:CG	2.53	0.43
1:I:292:TYR:HE1	1:I:335:MET:HE3	1.83	0.43
1:B:141:MET:HG2	1:B:228:GLY:HA2	2.00	0.43
1:E:278:CYS:O	1:E:332:GLY:HA3	2.18	0.43
1:O:105:THR:HB	1:O:211:LYS:HD2	2.00	0.43
1:O:105:THR:O	1:O:329:ARG:NH1	2.51	0.43
1:J:104:THR:HB	1:J:214:MET:HE3	2.00	0.43
1:L:108:LEU:HD12	1:L:154:PHE:CZ	2.52	0.43
1:A:173:GLU:OE2	1:K:80:ASP:N	2.52	0.43
1:N:349:LEU:CD1	1:P:349:LEU:HD22	2.47	0.43
1:S:308:PHE:HE1	1:S:322:ALA:HB1	1.84	0.43
1:I:335:MET:HE2	1:I:335:MET:HB2	1.84	0.43
1:O:128:LYS:HG3	1:O:240:ASN:OD1	2.19	0.43
1:B:324:VAL:C	1:B:325:LYS:HD3	2.43	0.43
1:L:104:THR:HB	1:L:214:MET:HE3	2.01	0.43
1:P:108:LEU:HD23	1:P:108:LEU:HA	1.66	0.43
1:O:286:PHE:N	1:O:351:ILE:HG22	2.33	0.43
1:Q:269:LYS:HD3	1:Q:274:TRP:CE2	2.54	0.43
1:A:135:ARG:HD2	1:A:185:ILE:HG21	2.00	0.43
1:A:173:GLU:OE1	1:K:240:ASN:HA	2.19	0.43
1:B:87:SER:HA	1:B:232:VAL:O	2.18	0.43
1:H:108:LEU:HD23	1:H:115:THR:HG21	2.00	0.43
1:I:108:LEU:HD23	1:I:108:LEU:HA	1.77	0.43
1:K:143:PRO:HB3	1:L:145:THR:O	2.19	0.43
1:T:145:THR:O	1:S:143:PRO:HB3	2.17	0.43
1:R:101:PRO:HA	1:R:217:TYR:HB3	2.01	0.43
1:R:108:LEU:HD23	1:R:108:LEU:HA	1.66	0.43
1:R:265:TRP:CZ3	1:R:278:CYS:HB2	2.54	0.43
1:E:80:ASP:CG	1:E:81:GLY:H	2.26	0.43
1:N:141:MET:HE3	1:O:149:LYS:HG3	2.01	0.43
1:C:250:ILE:HG12	1:C:347:GLN:HG3	2.00	0.42
1:F:301:GLU:HA	1:F:308:PHE:CE2	2.54	0.42
1:F:335:MET:HE2	1:F:335:MET:HB2	1.94	0.42
1:S:199:ASP:CG	1:S:201:ILE:HG13	2.44	0.42
1:A:349:LEU:HD12	1:F:349:LEU:HD13	2.00	0.42
1:I:302:ASN:HA	1:I:333:VAL:HG12	2.01	0.42
1:N:302:ASN:HA	1:N:333:VAL:HG12	2.00	0.42
1:O:349:LEU:HD23	1:O:350:ARG:C	2.44	0.42
1:B:269:LYS:HB2	1:B:274:TRP:CZ3	2.54	0.42
1:L:141:MET:HG2	1:L:228:GLY:HA2	2.01	0.42
1:R:326:VAL:HG13	1:R:331:GLN:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:SER:OG	1:B:277:ASP:HB2	2.19	0.42
1:K:149:LYS:NZ	1:O:139:SER:HB3	2.34	0.42
1:M:304:ASP:CG	1:M:331:GLN:HA	2.44	0.42
1:R:98:ASP:OD2	1:R:100:GLU:HB2	2.19	0.42
1:O:265:TRP:CH2	1:O:278:CYS:HB2	2.55	0.42
1:A:108:LEU:HD23	1:A:115:THR:HG21	2.01	0.42
1:E:306:SER:HB3	1:E:325:LYS:NZ	2.35	0.42
1:G:267:LYS:NZ	1:G:341:GLN:HG2	2.35	0.42
1:N:266:SER:OG	1:N:277:ASP:HB2	2.18	0.42
1:N:149:LYS:HG3	1:M:141:MET:HE3	2.02	0.42
1:M:108:LEU:HA	1:M:108:LEU:HD13	1.73	0.42
1:R:141:MET:HG2	1:R:228:GLY:HA2	2.01	0.42
1:Q:105:THR:HB	1:Q:211:LYS:HD2	2.00	0.42
1:B:94:LYS:HE2	1:B:226:GLN:HG2	2.02	0.42
1:G:304:ASP:CG	1:G:331:GLN:HA	2.45	0.42
1:B:326:VAL:HG13	1:B:331:GLN:HB2	2.01	0.42
1:B:335:MET:HE2	1:B:335:MET:HB2	1.85	0.42
1:E:105:THR:HB	1:E:211:LYS:HD2	2.01	0.42
1:F:87:SER:HA	1:F:232:VAL:O	2.20	0.42
1:J:82:ILE:HD11	1:J:238:LEU:HD12	2.01	0.42
1:K:292:TYR:HE2	1:K:314:ALA:HB1	1.85	0.42
1:M:266:SER:OG	1:M:277:ASP:HB2	2.20	0.42
1:P:250:ILE:HG12	1:P:347:GLN:HG3	2.01	0.42
1:R:307:ASP:HB3	1:R:325:LYS:HB3	2.01	0.42
1:H:283:THR:HG23	1:H:329:ARG:HG3	2.01	0.42
1:S:133:SER:HB3	1:S:235:THR:HB	2.02	0.42
1:Q:265:TRP:CZ3	1:Q:278:CYS:HB2	2.55	0.42
1:K:94:LYS:HE2	1:K:226:GLN:HG2	2.02	0.41
1:N:278:CYS:O	1:N:332:GLY:HA3	2.20	0.41
1:P:199:ASP:CG	1:P:201:ILE:HG13	2.45	0.41
1:A:84:ARG:HH22	1:F:241:ARG:HD3	1.85	0.41
1:A:149:LYS:HE3	1:E:139:SER:OG	2.19	0.41
1:G:265:TRP:CZ3	1:G:278:CYS:HB2	2.55	0.41
1:M:103:TYR:CE2	1:M:163:PRO:O	2.73	0.41
1:L:133:SER:HB3	1:L:235:THR:HB	2.02	0.41
1:P:335:MET:HE2	1:P:335:MET:HB2	1.84	0.41
1:R:312:GLY:HA3	1:R:320:GLN:HG2	2.02	0.41
1:D:108:LEU:CD1	1:D:134:LEU:HD21	2.51	0.41
1:H:351:ILE:OXT	1:H:351:ILE:HG22	2.20	0.41
1:I:144:SER:HA	1:I:181:TRP:CG	2.54	0.41
1:N:196:PHE:CD2	1:Q:205:LYS:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:128:LYS:HE3	1:L:196:PHE:CE2	2.55	0.41
1:P:167:ALA:HB1	1:T:117:ASN:HD22	1.84	0.41
1:P:179:VAL:HG23	1:P:182:THR:HB	2.01	0.41
1:T:101:PRO:HA	1:T:217:TYR:HB3	2.02	0.41
1:S:289:THR:HG22	1:S:321:TRP:CD1	2.56	0.41
1:A:113:PRO:HG3	1:A:261:ARG:O	2.21	0.41
1:D:289:THR:HG22	1:D:321:TRP:CD1	2.55	0.41
1:H:351:ILE:HD13	1:H:351:ILE:HA	1.94	0.41
1:J:103:TYR:CE2	1:J:163:PRO:O	2.74	0.41
1:M:125:GLN:HG2	1:M:244:SER:OG	2.19	0.41
1:T:335:MET:HE2	1:T:335:MET:HB2	1.93	0.41
1:D:101:PRO:HA	1:D:217:TYR:HB3	2.03	0.41
1:L:87:SER:HA	1:L:232:VAL:O	2.21	0.41
1:O:300:LEU:HD23	1:O:335:MET:HB3	2.03	0.41
1:Q:267:LYS:HG2	1:Q:274:TRP:CE3	2.55	0.41
1:H:135:ARG:HH21	1:H:185:ILE:HD13	1.86	0.41
1:N:113:PRO:HG3	1:N:261:ARG:O	2.21	0.41
1:N:289:THR:OG1	1:N:347:GLN:HB3	2.20	0.41
1:P:304:ASP:HB2	1:P:331:GLN:HA	2.03	0.41
1:D:335:MET:HE2	1:D:335:MET:HB2	1.90	0.41
1:F:131:PHE:CE1	1:F:236:VAL:HB	2.55	0.41
1:K:285:ASN:HB3	1:K:351:ILE:HG23	2.03	0.41
1:M:87:SER:HA	1:M:232:VAL:O	2.20	0.41
1:Q:141:MET:HG2	1:Q:228:GLY:HA2	2.02	0.41
1:C:292:TYR:HE2	1:C:335:MET:HE3	1.86	0.41
1:H:335:MET:HE2	1:H:335:MET:HB2	1.86	0.41
1:K:269:LYS:HD2	1:K:274:TRP:CZ2	2.55	0.41
1:N:292:TYR:HE1	1:N:335:MET:HE3	1.86	0.41
1:L:335:MET:HE2	1:L:335:MET:HB2	1.92	0.41
1:A:82:ILE:HD11	1:A:238:LEU:HD12	2.03	0.41
1:A:205:LYS:HB3	1:K:196:PHE:CD2	2.55	0.41
1:A:335:MET:HE2	1:A:335:MET:HB2	1.86	0.41
1:D:294:LYS:HE2	1:D:295:ALA:N	2.36	0.41
1:F:149:LYS:HB3	1:F:217:TYR:CE1	2.56	0.41
1:G:289:THR:HG21	1:O:289:THR:HG21	2.03	0.41
1:K:95:LYS:HA	1:K:227:LEU:HD11	2.02	0.41
1:M:292:TYR:CE1	1:M:296:PRO:HG3	2.56	0.41
1:M:329:ARG:H	1:M:329:ARG:HG2	1.39	0.41
1:M:335:MET:HB2	1:M:335:MET:HE2	1.85	0.41
1:P:94:LYS:HE2	1:P:226:GLN:HG2	2.02	0.41
1:Q:292:TYR:HE1	1:Q:335:MET:HE3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:TRP:CH2	1:E:278:CYS:HB2	2.54	0.41
1:R:121:LYS:HD3	1:R:121:LYS:HA	1.82	0.41
1:A:103:TYR:HE2	1:A:163:PRO:O	2.04	0.40
1:H:95:LYS:HA	1:H:227:LEU:HD11	2.03	0.40
1:H:266:SER:OG	1:H:277:ASP:HB2	2.21	0.40
1:C:108:LEU:HD23	1:C:108:LEU:HA	1.71	0.40
1:C:265:TRP:CZ3	1:C:278:CYS:HB2	2.56	0.40
1:A:205:LYS:HB3	1:K:196:PHE:HD2	1.86	0.40
1:C:136:PHE:HE2	1:C:154:PHE:CD1	2.39	0.40
1:C:274:TRP:CD1	1:C:340:GLU:HA	2.57	0.40
1:C:302:ASN:HA	1:C:333:VAL:HG12	2.03	0.40
1:J:103:TYR:CE1	1:J:215:ALA:HB2	2.57	0.40
1:P:166:LEU:HD11	1:P:217:TYR:CE2	2.56	0.40
1:O:114:GLY:HA2	1:O:282:GLY:HA2	2.03	0.40
1:O:136:PHE:CD2	1:O:212:LEU:HD22	2.57	0.40
1:O:266:SER:OG	1:O:277:ASP:HB2	2.20	0.40
1:B:135:ARG:HD2	1:B:185:ILE:HG21	2.04	0.40
1:D:87:SER:HA	1:D:232:VAL:O	2.21	0.40
1:T:276:HIS:HD2	1:T:335:MET:SD	2.44	0.40
1:R:302:ASN:HB2	1:R:308:PHE:CD2	2.57	0.40
1:C:306:SER:HB2	1:C:325:LYS:NZ	2.36	0.40
1:G:136:PHE:CD1	1:G:212:LEU:HD22	2.56	0.40
1:O:351:ILE:HG23	1:O:351:ILE:OXT	2.20	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	270/351 (77%)	260 (96%)	9 (3%)	1 (0%)	30 59
1	B	270/351 (77%)	261 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	270/351 (77%)	260 (96%)	10 (4%)	0	100	100
1	D	270/351 (77%)	260 (96%)	9 (3%)	1 (0%)	30	59
1	E	270/351 (77%)	259 (96%)	11 (4%)	0	100	100
1	F	270/351 (77%)	261 (97%)	9 (3%)	0	100	100
1	G	270/351 (77%)	260 (96%)	10 (4%)	0	100	100
1	H	270/351 (77%)	261 (97%)	9 (3%)	0	100	100
1	I	270/351 (77%)	261 (97%)	9 (3%)	0	100	100
1	J	270/351 (77%)	262 (97%)	8 (3%)	0	100	100
1	K	270/351 (77%)	261 (97%)	9 (3%)	0	100	100
1	L	270/351 (77%)	260 (96%)	10 (4%)	0	100	100
1	M	270/351 (77%)	259 (96%)	11 (4%)	0	100	100
1	N	270/351 (77%)	260 (96%)	10 (4%)	0	100	100
1	O	270/351 (77%)	260 (96%)	10 (4%)	0	100	100
1	P	270/351 (77%)	261 (97%)	9 (3%)	0	100	100
1	Q	270/351 (77%)	261 (97%)	9 (3%)	0	100	100
1	R	270/351 (77%)	260 (96%)	10 (4%)	0	100	100
1	S	270/351 (77%)	262 (97%)	8 (3%)	0	100	100
1	T	270/351 (77%)	260 (96%)	10 (4%)	0	100	100
All	All	5400/7020 (77%)	5209 (96%)	189 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	255	GLY
1	A	304	ASP

### 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	220/285 (77%)	213 (97%)	7 (3%)	34	68
1	B	220/285 (77%)	210 (96%)	10 (4%)	24	58
1	C	220/285 (77%)	210 (96%)	10 (4%)	24	58
1	D	220/285 (77%)	215 (98%)	5 (2%)	44	76
1	E	220/285 (77%)	212 (96%)	8 (4%)	31	65
1	F	220/285 (77%)	211 (96%)	9 (4%)	27	61
1	G	220/285 (77%)	213 (97%)	7 (3%)	34	68
1	H	220/285 (77%)	212 (96%)	8 (4%)	31	65
1	I	220/285 (77%)	211 (96%)	9 (4%)	27	61
1	J	220/285 (77%)	215 (98%)	5 (2%)	44	76
1	K	220/285 (77%)	211 (96%)	9 (4%)	27	61
1	L	220/285 (77%)	210 (96%)	10 (4%)	24	58
1	M	220/285 (77%)	208 (94%)	12 (6%)	19	50
1	N	220/285 (77%)	214 (97%)	6 (3%)	39	73
1	O	220/285 (77%)	212 (96%)	8 (4%)	31	65
1	P	220/285 (77%)	210 (96%)	10 (4%)	24	58
1	Q	220/285 (77%)	211 (96%)	9 (4%)	27	61
1	R	220/285 (77%)	214 (97%)	6 (3%)	39	73
1	S	220/285 (77%)	213 (97%)	7 (3%)	34	68
1	T	220/285 (77%)	210 (96%)	10 (4%)	24	58
All	All	4400/5700 (77%)	4235 (96%)	165 (4%)	29	64

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	THR
1	A	141	MET
1	A	179	VAL
1	A	217	TYR
1	A	232	VAL
1	A	289	THR
1	A	339	GLU
1	B	104	THR
1	B	122	GLU
1	B	128	LYS
1	B	141	MET

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Mol	Chain	Res	Type
1	B	179	VAL
1	B	201	ILE
1	B	232	VAL
1	B	294	LYS
1	B	325	LYS
1	B	349	LEU
1	C	104	THR
1	C	128	LYS
1	C	141	MET
1	C	156	ARG
1	C	176	VAL
1	C	179	VAL
1	C	232	VAL
1	C	306	SER
1	C	339	GLU
1	C	351	ILE
1	D	104	THR
1	D	232	VAL
1	D	241	ARG
1	D	294	LYS
1	D	304	ASP
1	E	104	THR
1	E	179	VAL
1	E	232	VAL
1	E	261	ARG
1	E	301	GLU
1	E	339	GLU
1	E	349	LEU
1	E	351	ILE
1	F	84	ARG
1	F	98	ASP
1	F	122	GLU
1	F	128	LYS
1	F	179	VAL
1	F	232	VAL
1	F	233	GLU
1	F	239	LYS
1	F	349	LEU
1	G	104	THR
1	G	141	MET
1	G	179	VAL
1	G	201	ILE

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Mol	Chain	Res	Type
1	G	232	VAL
1	G	245	THR
1	G	247	ASP
1	H	84	ARG
1	H	104	THR
1	H	128	LYS
1	H	141	MET
1	H	179	VAL
1	H	201	ILE
1	H	232	VAL
1	H	339	GLU
1	I	104	THR
1	I	128	LYS
1	I	141	MET
1	I	179	VAL
1	I	201	ILE
1	I	232	VAL
1	I	239	LYS
1	I	339	GLU
1	I	349	LEU
1	J	104	THR
1	J	141	MET
1	J	176	VAL
1	J	179	VAL
1	J	232	VAL
1	K	100	GLU
1	K	104	THR
1	K	137	ARG
1	K	179	VAL
1	K	201	ILE
1	K	232	VAL
1	K	239	LYS
1	K	339	GLU
1	K	351	ILE
1	N	104	THR
1	N	122	GLU
1	N	179	VAL
1	N	217	TYR
1	N	232	VAL
1	N	241	ARG
1	M	98	ASP
1	M	104	THR

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Mol	Chain	Res	Type
1	M	108	LEU
1	M	128	LYS
1	M	141	MET
1	M	179	VAL
1	M	201	ILE
1	M	232	VAL
1	M	261	ARG
1	M	301	GLU
1	M	329	ARG
1	M	351	ILE
1	L	104	THR
1	L	128	LYS
1	L	141	MET
1	L	168	SER
1	L	179	VAL
1	L	201	ILE
1	L	232	VAL
1	L	339	GLU
1	L	343	LYS
1	L	351	ILE
1	P	104	THR
1	P	134	LEU
1	P	141	MET
1	P	179	VAL
1	P	201	ILE
1	P	217	TYR
1	P	232	VAL
1	P	239	LYS
1	P	289	THR
1	P	334	LYS
1	O	84	ARG
1	O	104	THR
1	O	139	SER
1	O	141	MET
1	O	179	VAL
1	O	201	ILE
1	O	232	VAL
1	O	339	GLU
1	T	133	SER
1	T	141	MET
1	T	199	ASP
1	T	201	ILE

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Mol	Chain	Res	Type
1	T	232	VAL
1	T	245	THR
1	T	304	ASP
1	T	309	SER
1	T	339	GLU
1	T	349	LEU
1	S	104	THR
1	S	179	VAL
1	S	201	ILE
1	S	232	VAL
1	S	289	THR
1	S	304	ASP
1	S	339	GLU
1	R	104	THR
1	R	141	MET
1	R	179	VAL
1	R	217	TYR
1	R	232	VAL
1	R	241	ARG
1	Q	80	ASP
1	Q	104	THR
1	Q	141	MET
1	Q	156	ARG
1	Q	179	VAL
1	Q	201	ILE
1	Q	232	VAL
1	Q	277	ASP
1	Q	339	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	276	HIS
1	B	96	ASN
1	C	117	ASN
1	D	171	ASN
1	D	279	HIS
1	D	347	GLN
1	E	117	ASN
1	E	164	ASN
1	E	226	GLN

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Mol	Chain	Res	Type
1	F	118	GLN
1	F	240	ASN
1	G	226	GLN
1	H	226	GLN
1	H	240	ASN
1	I	171	ASN
1	J	240	ASN
1	K	240	ASN
1	N	96	ASN
1	N	285	ASN
1	M	226	GLN
1	L	240	ASN
1	L	276	HIS
1	P	240	ASN
1	O	285	ASN
1	T	240	ASN
1	R	117	ASN
1	R	240	ASN
1	Q	279	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	272/351 (77%)	-1.49	0 100 100	45, 62, 91, 108	0
1	B	272/351 (77%)	-1.41	0 100 100	41, 65, 136, 161	0
1	C	272/351 (77%)	-1.42	0 100 100	43, 63, 117, 131	0
1	D	272/351 (77%)	-1.43	0 100 100	43, 66, 125, 145	0
1	E	272/351 (77%)	-1.46	0 100 100	44, 65, 119, 134	0
1	F	272/351 (77%)	-1.48	0 100 100	40, 61, 98, 123	0
1	G	272/351 (77%)	-1.44	0 100 100	42, 68, 121, 136	0
1	H	272/351 (77%)	-1.46	0 100 100	38, 66, 122, 140	0
1	I	272/351 (77%)	-1.50	0 100 100	38, 59, 127, 137	0
1	J	272/351 (77%)	-1.39	0 100 100	38, 62, 124, 141	0
1	K	272/351 (77%)	-1.47	0 100 100	38, 65, 120, 136	0
1	L	272/351 (77%)	-1.44	0 100 100	40, 64, 143, 161	0
1	M	272/351 (77%)	-1.41	0 100 100	41, 62, 133, 154	0
1	N	272/351 (77%)	-1.52	0 100 100	44, 62, 116, 127	0
1	O	272/351 (77%)	-1.45	0 100 100	41, 67, 120, 135	0
1	P	272/351 (77%)	-1.46	0 100 100	43, 62, 116, 127	0
1	Q	272/351 (77%)	-1.45	0 100 100	41, 63, 121, 140	0
1	R	272/351 (77%)	-1.52	0 100 100	41, 61, 106, 132	0
1	S	272/351 (77%)	-1.53	0 100 100	34, 56, 87, 100	0
1	T	272/351 (77%)	-1.48	0 100 100	39, 61, 107, 117	0
All	All	5440/7020 (77%)	-1.46	0 100 100	34, 63, 123, 161	0

There are no RSRZ outliers to report.

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.