



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:27 PM UTC

PDB ID : 7F8I / pdb_00007f8i
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

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	:	4-5-2 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

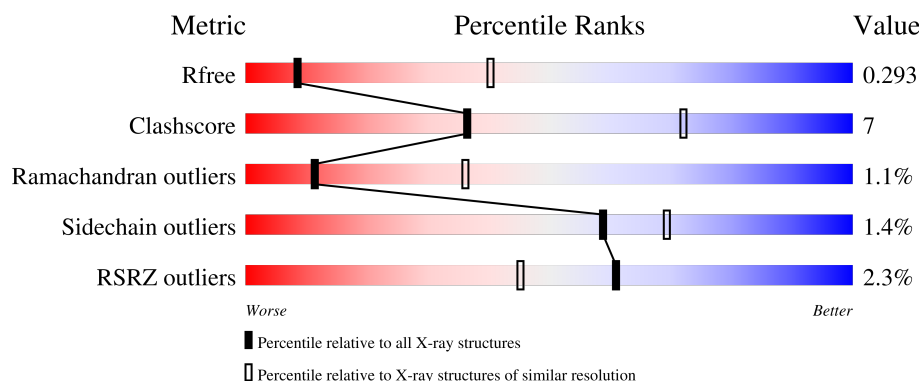
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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 $\leq 5\%$. 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	0% 67% 16% • 16%
1	B	496	2% 70% 12% • 17%
1	C	496	2% 68% 15% • 16%
1	D	496	2% 68% 15% 17%
1	E	496	3% 67% 16% • 16%

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Mol	Chain	Length	Quality of chain
1	F	496	3% 67% 15% • 18%
1	G	496	2% 69% 15% • 16%
1	H	496	% 68% 16% • 16%
1	I	496	2% 65% 16% • 18%
1	J	496	% 67% 15% • 16%

2 Entry composition

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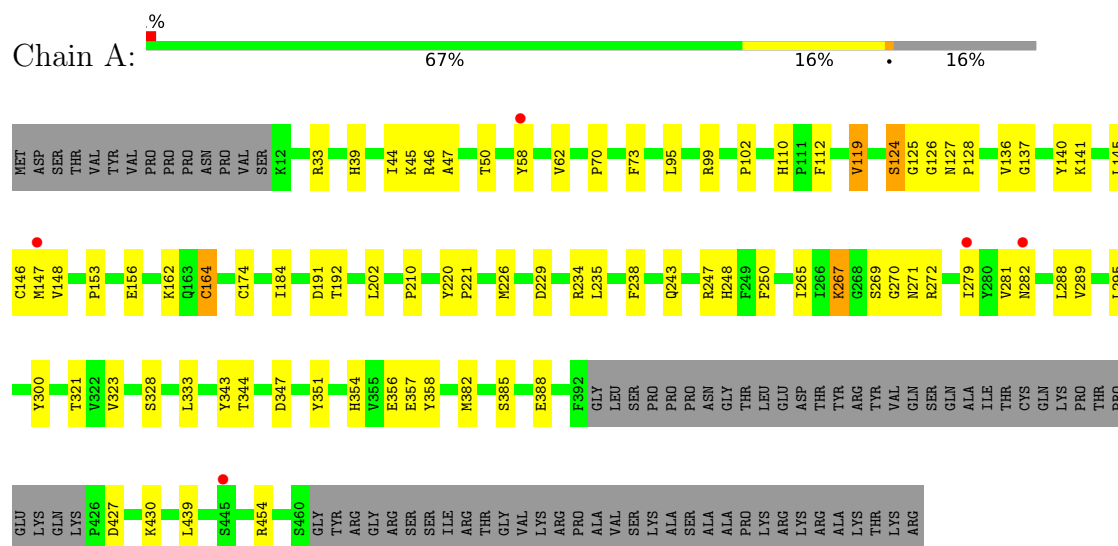
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Chain	Residue	Modelled	Actual	Comment	Reference
E	376	VAL	MET	conflict	UNP Q9W9C6
F	-2	MET	-	initiating methionine	UNP Q9W9C6
F	376	VAL	MET	conflict	UNP Q9W9C6
G	-2	MET	-	initiating methionine	UNP Q9W9C6
G	376	VAL	MET	conflict	UNP Q9W9C6
H	-2	MET	-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

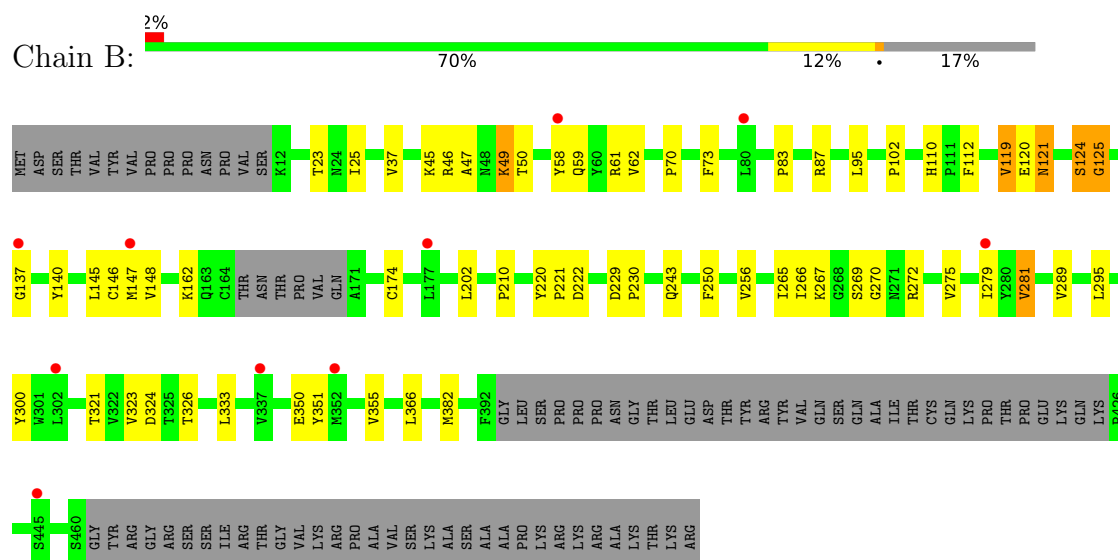
3 Residue-property plots [i](#)

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

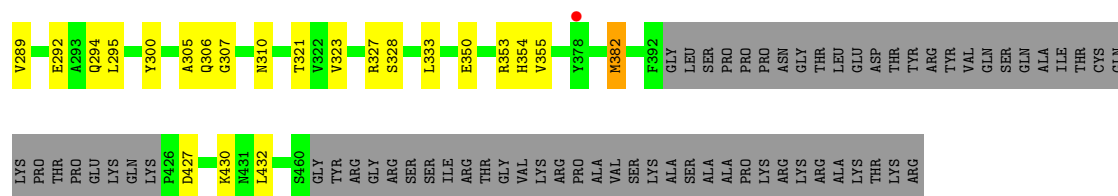


• Molecule 1: Major capsid protein L1

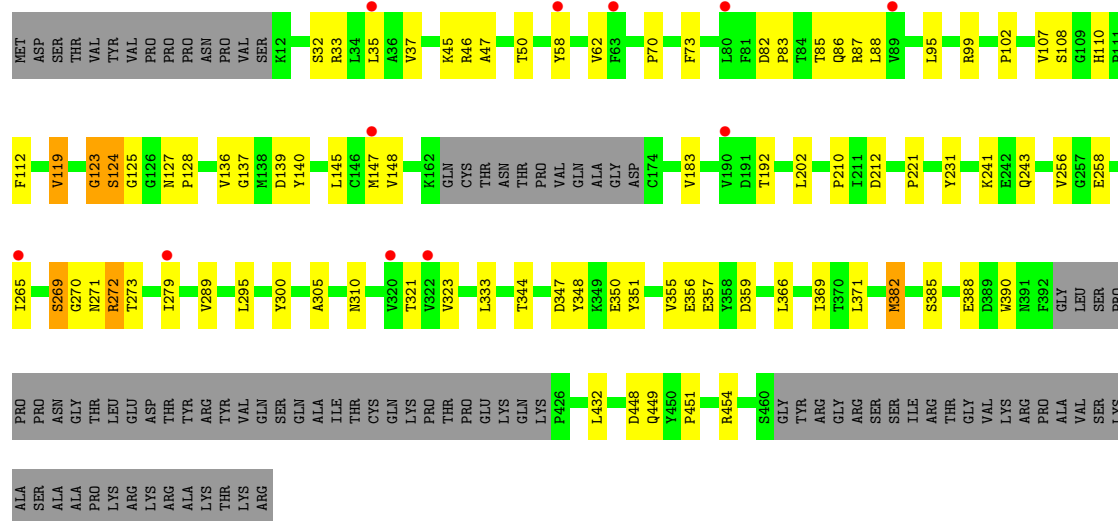


• Molecule 1: Major capsid protein L1

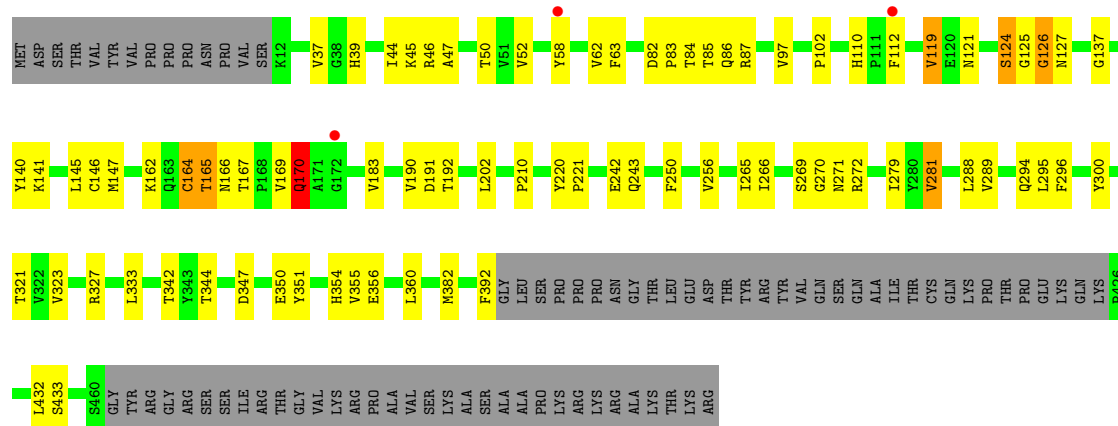




• Molecule 1: Major capsid protein L1



• 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, α , β , γ	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) 94.3 (33.88-3.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.256 , 0.294 0.254 , 0.293	Depositor DCC
R_{free} test set	3592 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	95.6	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	32368	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.13	0/3342	0.38	0/4544
1	B	0.13	0/3295	0.37	0/4476
1	C	0.11	0/3342	0.35	0/4544
1	D	0.11	0/3298	0.34	0/4480
1	E	0.11	0/3342	0.36	0/4544
1	F	0.11	0/3276	0.34	0/4452
1	G	0.12	0/3359	0.36	0/4567
1	H	0.13	0/3342	0.36	0/4544
1	I	0.13	0/3263	0.36	2/4433 (0.0%)
1	J	0.11	0/3342	0.35	0/4544
All	All	0.12	0/33201	0.36	2/45128 (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	F	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	124	SER	CA-C-N	5.10	130.87	121.70
1	I	124	SER	C-N-CA	5.10	130.87	121.70

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 [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	3258	0	3150	64	0
1	B	3213	0	3105	52	0
1	C	3258	0	3150	58	0
1	D	3216	0	3108	60	0
1	E	3258	0	3150	59	0
1	F	3194	0	3084	60	0
1	G	3274	0	3162	54	0
1	H	3258	0	3150	53	0
1	I	3181	0	3080	59	0
1	J	3258	0	3150	55	0
All	All	32368	0	31289	461	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 (461) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:147:MET:HE1	1:G:221:PRO:HB3	1.78	0.64
1:F:147:MET:HE1	1:F:221:PRO:HB3	1.80	0.63
1:A:145:LEU:HD13	1:A:147:MET:HE3	1.81	0.63
1:A:202:LEU:HB3	1:B:333:LEU:HD22	1.80	0.63
1:A:267:LYS:NZ	1:E:374:GLU:OE1	2.29	0.63
1:A:333:LEU:HD22	1:H:202:LEU:HB3	1.80	0.63
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:C:110:HIS:HB2	1:C:210:PRO:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:MET:HE1	1:A:221:PRO:HB3	1.83	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:H:147:MET:HE1	1:H:221:PRO:HB3	1.81	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
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:C:147:MET:HE1	1:C:221:PRO:HB3	1.84	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:147:MET:HE1	1:E:221:PRO:HB3	1.85	0.59
1:I:147:MET:HE1	1:I:221:PRO:HB3	1.84	0.59
1:A:141:LYS:NZ	1:A:191:ASP:OD2	2.25	0.59
1:E:45:LYS:HB3	1:E:50:THR:HA	1.84	0.59
1:J:145:LEU:HD13	1:J:147:MET:HE3	1.85	0.58
1:B:256:VAL:HA	1:B:279:ILE:HD11	1.85	0.58
1:C:145:LEU:HD13	1:C:147:MET:HE3	1.83	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:J:147:MET:HE1	1:J:221:PRO:HB3	1.84	0.57
1:G:202:LEU:HB3	1:J:333:LEU:HD22	1.87	0.57
1:F:110:HIS:HB2	1:F:210:PRO:HA	1.86	0.57
1:D:147:MET:HE1	1:D:221:PRO:HB3	1.85	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:H:124:SER:HB3	1:H:125:GLY:C	2.30	0.57
1:D:110:HIS:HB2	1:D:210:PRO:HA	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:145:LEU:HD13	1:I:147:MET:HE3	1.88	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:H:141:LYS:NZ	1:H:191:ASP:OD2	2.31	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:B:145:LEU:HD13	1:B:147:MET:HE3	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
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:G:269:SER:OG	1:G:270:GLY:N	2.32	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:B:62:VAL:HG22	1:B:321:THR:HG23	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:E:141:LYS:NZ	1:E:191:ASP:OD2	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:147:MET:HE1	1:A:221:PRO:CB	2.42	0.48
1:A:272:ARG:HD2	1:B:112:PHE:CE1	2.41	0.48
1:C:356:GLU:HB3	1:C:358:TYR:HE2	1.79	0.48
1:I:269:SER:OG	1:I:270:GLY:N	2.43	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: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:B:269:SER:OG	1:B:270:GLY:N	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:147:MET:HE1	1:C:221:PRO:CB	2.45	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:H:127:ASN:CG	1:H:128:PRO:HD2	2.40	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
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:G:162:LYS:C	1:G:164:CYS:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:108:SER:OG	1:D:212:ASP:OD2	2.33	0.45
1:I:82:ASP:O	1:I:86:GLN:HB2	2.16	0.45
1:J:162:LYS:C	1:J:164:CYS:H	2.24	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: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:D:147:MET:HE1	1:D:221:PRO:CB	2.47	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
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:H:270:GLY:C	1:H:272:ARG:H	2.22	0.44
1:I:147:MET:HE1	1:I:221:PRO:CB	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:84:THR:O	1:F:85:THR:OG1	2.32	0.43
1:G:161:GLY:HA2	1:G:178:GLU:CD	2.42	0.43
1:B:324:ASP:OD1	1:B:326:THR:OG1	2.32	0.43
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:H:292:GLU:OE2	1:I:241:LYS:NZ	2.47	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:F:147:MET:HE1	1:F:221:PRO:CB	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:145:LEU:HD13	1:F:147:MET:HE3	2.00	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:B:23:THR:OG1	1:B:366:LEU:O	2.34	0.42
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:G:459:GLN:C	1:G:461:GLY:H	2.26	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:I:108:SER:OG	1:I:212:ASP:OD2	2.35	0.42
1:A:238:PHE:CD1	1:A:238:PHE:C	2.97	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: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:B:147:MET:HE1	1:B:221:PRO:CB	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:238:PHE:CD1	1:C:238:PHE:C	2.98	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:B:120:GLU:C	1:B:121:ASN:OD1	2.64	0.41
1:C:121:ASN:OD1	1:C:121:ASN:N	2.54	0.41
1:E:84:THR:O	1:E:85:THR:OG1	2.33	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:H:99:ARG:HA	1:H:99:ARG:HD2	1.90	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:J:169:VAL:O	1:J:170:GLN:C	2.63	0.40
1:C:84:THR:O	1:C:85:THR:OG1	2.32	0.40
1:E:119:VAL:HG12	1:E:249:PHE:CB	2.52	0.40
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/496 (83%)	389 (94%)	19 (5%)	4 (1%)	12	38
1	B	404/496 (82%)	385 (95%)	15 (4%)	4 (1%)	12	38
1	C	412/496 (83%)	391 (95%)	15 (4%)	6 (2%)	8	29
1	D	404/496 (82%)	387 (96%)	15 (4%)	2 (0%)	24	52
1	E	412/496 (83%)	390 (95%)	18 (4%)	4 (1%)	12	38
1	F	401/496 (81%)	382 (95%)	15 (4%)	4 (1%)	12	38
1	G	414/496 (84%)	391 (94%)	19 (5%)	4 (1%)	12	38
1	H	412/496 (83%)	393 (95%)	15 (4%)	4 (1%)	12	38
1	I	399/496 (80%)	382 (96%)	12 (3%)	5 (1%)	9	32
1	J	412/496 (83%)	388 (94%)	17 (4%)	7 (2%)	7	27
All	All	4082/4960 (82%)	3878 (95%)	160 (4%)	44 (1%)	11	36

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
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

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Mol	Chain	Res	Type
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%)	73 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	357/432 (83%)	350 (98%)	7 (2%)	48	65
1	C	363/432 (84%)	358 (99%)	5 (1%)	59	69
1	D	357/432 (83%)	353 (99%)	4 (1%)	65	73
1	E	363/432 (84%)	358 (99%)	5 (1%)	59	69
1	F	355/432 (82%)	353 (99%)	2 (1%)	78	79
1	G	364/432 (84%)	358 (98%)	6 (2%)	55	67
1	H	363/432 (84%)	357 (98%)	6 (2%)	53	67
1	I	354/432 (82%)	350 (99%)	4 (1%)	65	73
1	J	363/432 (84%)	356 (98%)	7 (2%)	50	66
All	All	3602/4320 (83%)	3553 (99%)	49 (1%)	59	69

All (49) 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	49	LYS
1	B	119	VAL
1	B	121	ASN
1	B	162	LYS
1	B	229	ASP
1	B	267	LYS
1	B	281	VAL
1	C	49	LYS
1	C	119	VAL
1	C	127	ASN
1	C	267	LYS
1	C	281	VAL
1	D	46	ARG
1	D	49	LYS
1	D	267	LYS
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

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Mol	Chain	Res	Type
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	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	35	LEU
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	281	VAL
1	J	288	LEU
1	J	433	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	C	365	GLN
1	D	243	GLN
1	E	28	HIS
1	E	157	HIS
1	E	243	GLN
1	F	28	HIS
1	F	144	GLN
1	F	248	HIS
1	G	243	GLN
1	H	306	GLN
1	I	185	GLN
1	I	365	GLN
1	J	142	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	416/496 (83%)	-0.06	5 (1%) 76 63	47, 73, 124, 205	0
1	B	410/496 (82%)	0.02	10 (2%) 59 44	56, 87, 150, 194	0
1	C	416/496 (83%)	-0.04	8 (1%) 66 49	67, 99, 168, 259	0
1	D	410/496 (82%)	0.06	12 (2%) 53 39	64, 88, 139, 190	0
1	E	416/496 (83%)	0.05	15 (3%) 46 33	70, 93, 152, 222	0
1	F	407/496 (82%)	0.08	17 (4%) 40 28	67, 117, 175, 226	0
1	G	418/496 (84%)	0.06	9 (2%) 62 46	68, 104, 163, 232	0
1	H	416/496 (83%)	0.07	7 (1%) 69 53	62, 103, 161, 236	0
1	I	405/496 (81%)	0.27	11 (2%) 56 41	73, 126, 190, 225	0
1	J	416/496 (83%)	0.01	3 (0%) 84 73	75, 105, 162, 213	0
All	All	4130/4960 (83%)	0.05	97 (2%) 61 45	47, 99, 164, 259	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	MET	5.6
1	H	58	TYR	5.3
1	B	58	TYR	4.6
1	F	58	TYR	4.4
1	E	58	TYR	4.1
1	J	58	TYR	4.0
1	I	80	LEU	4.0
1	I	58	TYR	3.8
1	D	114	ASN	3.8
1	B	302	LEU	3.4
1	D	58	TYR	3.3
1	E	147	MET	3.3
1	E	94	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	270	GLY	3.2
1	A	58	TYR	3.1
1	H	70	PRO	3.1
1	A	279	ILE	3.1
1	G	112	PHE	3.1
1	I	279	ILE	3.1
1	I	322	VAL	3.0
1	F	80	LEU	3.0
1	E	208	ASP	3.0
1	D	368	SER	3.0
1	G	204	THR	3.0
1	F	112	PHE	2.9
1	D	208	ASP	2.9
1	B	337	VAL	2.9
1	H	97	VAL	2.8
1	I	265	ILE	2.8
1	H	147	MET	2.8
1	F	237	PHE	2.7
1	F	236	PHE	2.7
1	F	215	GLY	2.7
1	A	445	SER	2.7
1	D	355	VAL	2.7
1	E	279	ILE	2.6
1	C	215	GLY	2.6
1	D	254	GLY	2.6
1	B	445	SER	2.5
1	B	137	GLY	2.5
1	E	282	ASN	2.5
1	C	58	TYR	2.5
1	F	172	GLY	2.5
1	B	279	ILE	2.4
1	H	80	LEU	2.4
1	I	147	MET	2.4
1	C	30	SER	2.4
1	E	150	CYS	2.4
1	J	172	GLY	2.4
1	D	147	MET	2.4
1	F	204	THR	2.4
1	F	282	ASN	2.4
1	I	320	VAL	2.4
1	E	215	GLY	2.4
1	E	262	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	63	PHE	2.4
1	G	147	MET	2.3
1	D	235	LEU	2.3
1	E	258	GLU	2.3
1	F	192	THR	2.3
1	B	352	MET	2.3
1	I	89	VAL	2.3
1	E	177	LEU	2.3
1	J	112	PHE	2.3
1	F	369	ILE	2.3
1	C	147	MET	2.3
1	G	306	GLN	2.3
1	F	352	MET	2.3
1	F	201	ASP	2.3
1	G	282	ASN	2.2
1	B	80	LEU	2.2
1	G	253	ALA	2.2
1	A	147	MET	2.2
1	F	355	VAL	2.2
1	D	150	CYS	2.2
1	F	113	LEU	2.1
1	D	279	ILE	2.1
1	D	429	TYR	2.1
1	G	235	LEU	2.1
1	A	282	ASN	2.1
1	F	147	MET	2.1
1	C	172	GLY	2.1
1	E	270	GLY	2.1
1	H	281	VAL	2.1
1	I	190	VAL	2.1
1	G	21	THR	2.1
1	E	126	GLY	2.1
1	B	177	LEU	2.1
1	E	172	GLY	2.1
1	C	282	ASN	2.0
1	I	35	LEU	2.0
1	E	63	PHE	2.0
1	F	306	GLN	2.0
1	G	137	GLY	2.0
1	H	378	TYR	2.0
1	C	191	ASP	2.0
1	C	137	GLY	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 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.