



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:08 PM UTC

PDB ID : 4RS5 / pdb_00004rs5
Title : Crystal structure of an uncoating intermediate of a EV71 recombinant virus
Authors : Chen, R.; Lyu, K.
Deposited on : 2014-11-07
Resolution : 3.81 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

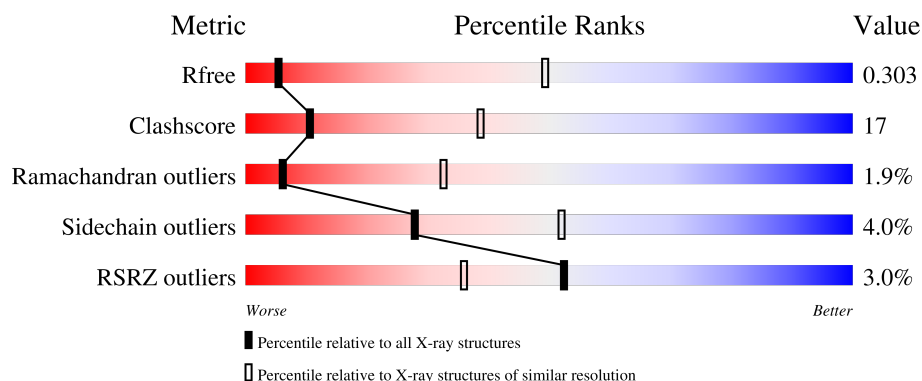
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	B	242	
1	E	242	
1	H	242	
1	K	242	
1	N	242	

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Mol	Chain	Length	Quality of chain
2	C	323	
2	F	323	
2	I	323	
2	L	323	
2	O	323	
3	A	313	
3	D	313	
3	G	313	
3	J	313	
3	M	313	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26425 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 VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	223	Total	C	N	O	S	0	0	0
			1699	1093	279	316	11			
1	N	223	Total	C	N	O	S	0	0	0
			1699	1093	279	316	11			
1	B	223	Total	C	N	O	S	0	0	0
			1699	1093	279	316	11			
1	H	223	Total	C	N	O	S	0	0	0
			1699	1093	279	316	11			
1	K	223	Total	C	N	O	S	0	0	0
			1699	1093	279	316	11			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	227	GLN	LYS	engineered mutation	UNP F6KTB0
N	227	GLN	LYS	engineered mutation	UNP F6KTB0
B	227	GLN	LYS	engineered mutation	UNP F6KTB0
H	227	GLN	LYS	engineered mutation	UNP F6KTB0
K	227	GLN	LYS	engineered mutation	UNP F6KTB0

- Molecule 2 is a protein called Capsid protein VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	236	Total	C	N	O	S	0	0	0
			1829	1174	303	344	8			
2	O	236	Total	C	N	O	S	0	0	0
			1829	1174	303	344	8			
2	C	236	Total	C	N	O	S	0	0	0
			1829	1174	303	344	8			
2	I	236	Total	C	N	O	S	0	0	0
			1829	1174	303	344	8			
2	L	236	Total	C	N	O	S	0	0	0
			1829	1174	303	344	8			

- Molecule 3 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	221	Total	C	N	O	S	0	0	0
			1757	1128	295	323	11			
3	M	221	Total	C	N	O	S	0	0	0
			1757	1128	295	323	11			
3	A	221	Total	C	N	O	S	0	0	0
			1757	1128	295	323	11			
3	G	221	Total	C	N	O	S	0	0	0
			1757	1128	295	323	11			
3	J	221	Total	C	N	O	S	0	0	0
			1757	1128	295	323	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	101	SER	-	insertion	UNP F6KTB0
D	102	VAL	-	insertion	UNP F6KTB0
D	103	LYS	-	insertion	UNP F6KTB0
D	104	ARG	-	insertion	UNP F6KTB0
D	105	GLY	-	insertion	UNP F6KTB0
D	106	THR	-	insertion	UNP F6KTB0
D	107	SER	-	insertion	UNP F6KTB0
D	108	VAL	-	insertion	UNP F6KTB0
D	109	GLY	-	insertion	UNP F6KTB0
D	110	MET	-	insertion	UNP F6KTB0
D	111	LYS	-	insertion	UNP F6KTB0
D	112	PRO	-	insertion	UNP F6KTB0
D	113	SER	-	insertion	UNP F6KTB0
D	114	PRO	-	insertion	UNP F6KTB0
D	115	ARG	-	insertion	UNP F6KTB0
D	116	PRO	-	insertion	UNP F6KTB0
M	101	SER	-	insertion	UNP F6KTB0
M	102	VAL	-	insertion	UNP F6KTB0
M	103	LYS	-	insertion	UNP F6KTB0
M	104	ARG	-	insertion	UNP F6KTB0
M	105	GLY	-	insertion	UNP F6KTB0
M	106	THR	-	insertion	UNP F6KTB0
M	107	SER	-	insertion	UNP F6KTB0
M	108	VAL	-	insertion	UNP F6KTB0
M	109	GLY	-	insertion	UNP F6KTB0
M	110	MET	-	insertion	UNP F6KTB0
M	111	LYS	-	insertion	UNP F6KTB0
M	112	PRO	-	insertion	UNP F6KTB0

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Chain	Residue	Modelled	Actual	Comment	Reference
M	113	SER	-	insertion	UNP F6KTB0
M	114	PRO	-	insertion	UNP F6KTB0
M	115	ARG	-	insertion	UNP F6KTB0
M	116	PRO	-	insertion	UNP F6KTB0
A	101	SER	-	insertion	UNP F6KTB0
A	102	VAL	-	insertion	UNP F6KTB0
A	103	LYS	-	insertion	UNP F6KTB0
A	104	ARG	-	insertion	UNP F6KTB0
A	105	GLY	-	insertion	UNP F6KTB0
A	106	THR	-	insertion	UNP F6KTB0
A	107	SER	-	insertion	UNP F6KTB0
A	108	VAL	-	insertion	UNP F6KTB0
A	109	GLY	-	insertion	UNP F6KTB0
A	110	MET	-	insertion	UNP F6KTB0
A	111	LYS	-	insertion	UNP F6KTB0
A	112	PRO	-	insertion	UNP F6KTB0
A	113	SER	-	insertion	UNP F6KTB0
A	114	PRO	-	insertion	UNP F6KTB0
A	115	ARG	-	insertion	UNP F6KTB0
A	116	PRO	-	insertion	UNP F6KTB0
G	101	SER	-	insertion	UNP F6KTB0
G	102	VAL	-	insertion	UNP F6KTB0
G	103	LYS	-	insertion	UNP F6KTB0
G	104	ARG	-	insertion	UNP F6KTB0
G	105	GLY	-	insertion	UNP F6KTB0
G	106	THR	-	insertion	UNP F6KTB0
G	107	SER	-	insertion	UNP F6KTB0
G	108	VAL	-	insertion	UNP F6KTB0
G	109	GLY	-	insertion	UNP F6KTB0
G	110	MET	-	insertion	UNP F6KTB0
G	111	LYS	-	insertion	UNP F6KTB0
G	112	PRO	-	insertion	UNP F6KTB0
G	113	SER	-	insertion	UNP F6KTB0
G	114	PRO	-	insertion	UNP F6KTB0
G	115	ARG	-	insertion	UNP F6KTB0
G	116	PRO	-	insertion	UNP F6KTB0
J	101	SER	-	insertion	UNP F6KTB0
J	102	VAL	-	insertion	UNP F6KTB0
J	103	LYS	-	insertion	UNP F6KTB0
J	104	ARG	-	insertion	UNP F6KTB0
J	105	GLY	-	insertion	UNP F6KTB0
J	106	THR	-	insertion	UNP F6KTB0

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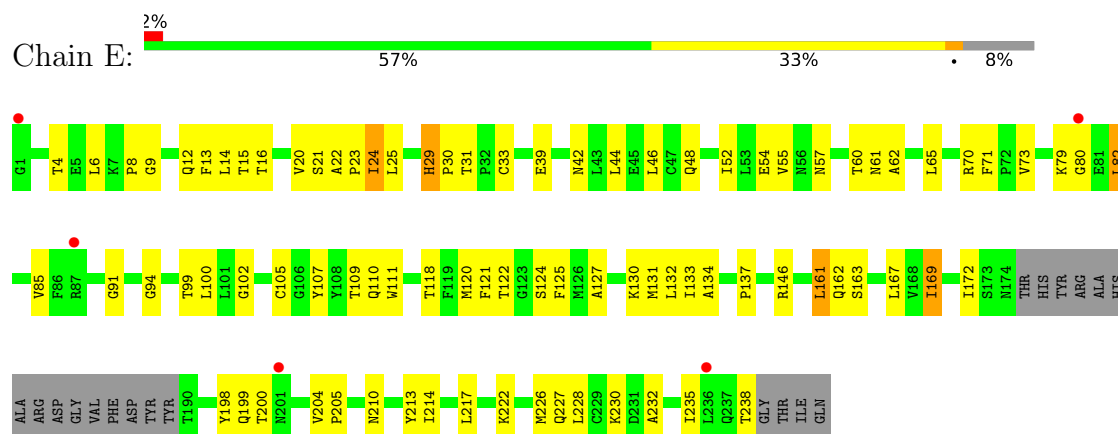
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Chain	Residue	Modelled	Actual	Comment	Reference
J	107	SER	-	insertion	UNP F6KTB0
J	108	VAL	-	insertion	UNP F6KTB0
J	109	GLY	-	insertion	UNP F6KTB0
J	110	MET	-	insertion	UNP F6KTB0
J	111	LYS	-	insertion	UNP F6KTB0
J	112	PRO	-	insertion	UNP F6KTB0
J	113	SER	-	insertion	UNP F6KTB0
J	114	PRO	-	insertion	UNP F6KTB0
J	115	ARG	-	insertion	UNP F6KTB0
J	116	PRO	-	insertion	UNP F6KTB0

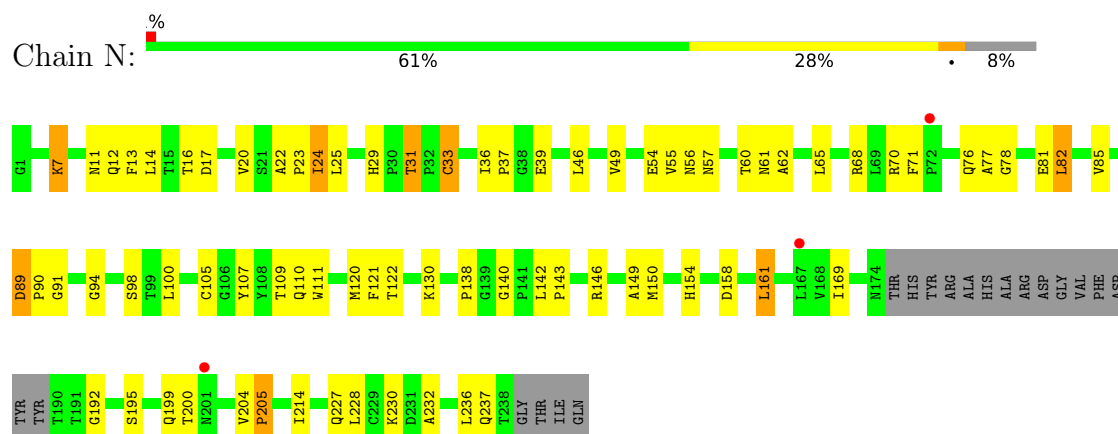
3 Residue-property plots

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.

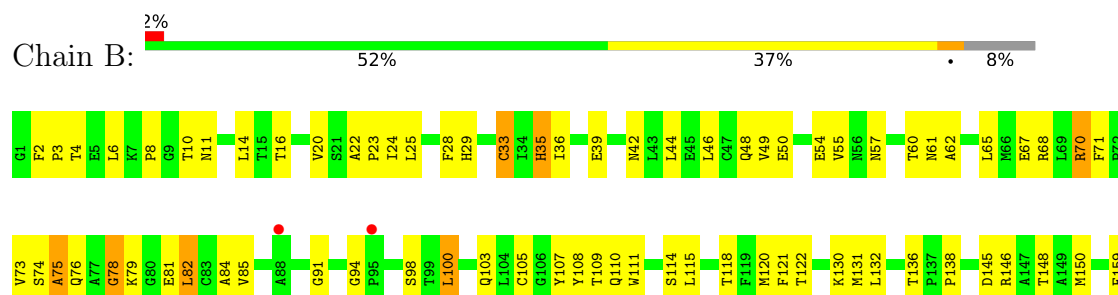
• Molecule 1: Capsid protein VP3

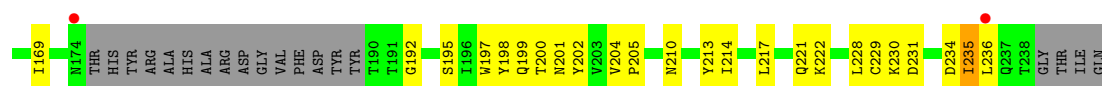


• Molecule 1: Capsid protein VP3

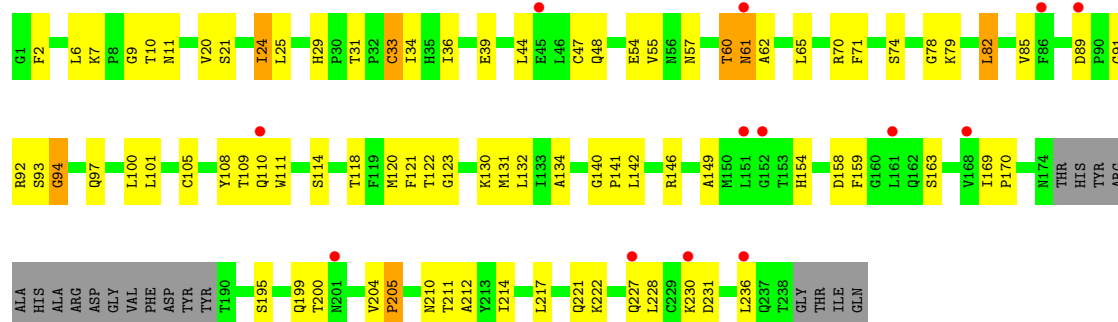


• Molecule 1: Capsid protein VP3

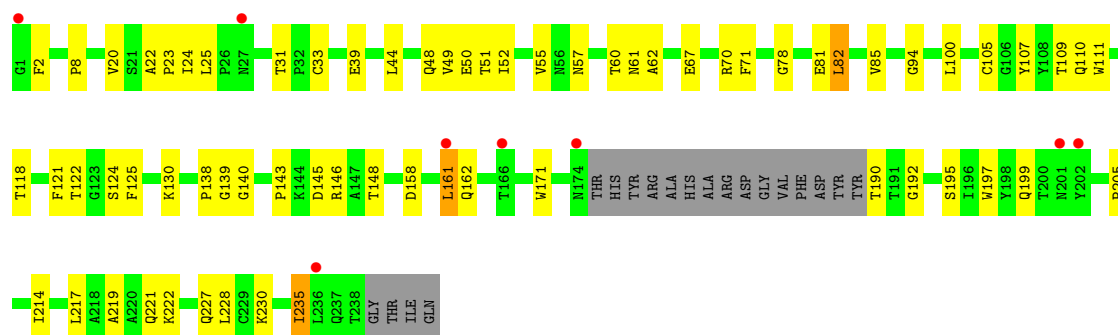




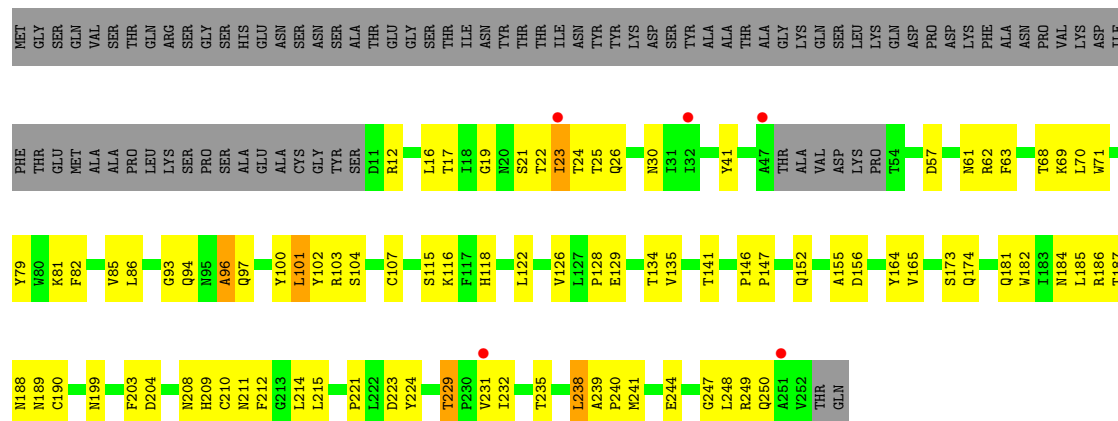
• Molecule 1: Capsid protein VP3



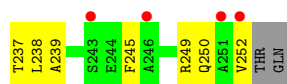
• Molecule 1: Capsid protein VP3



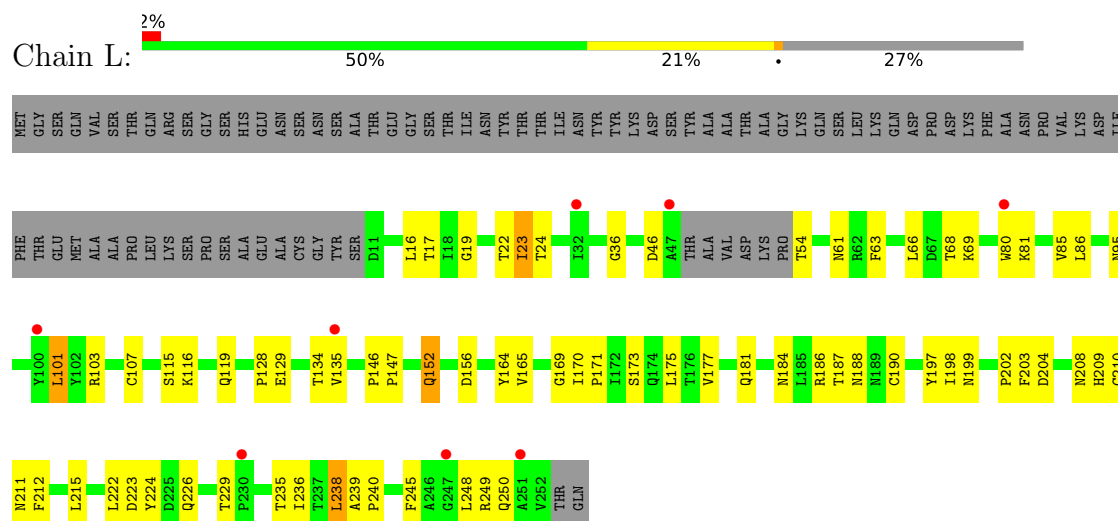
• Molecule 2: Capsid protein VP0



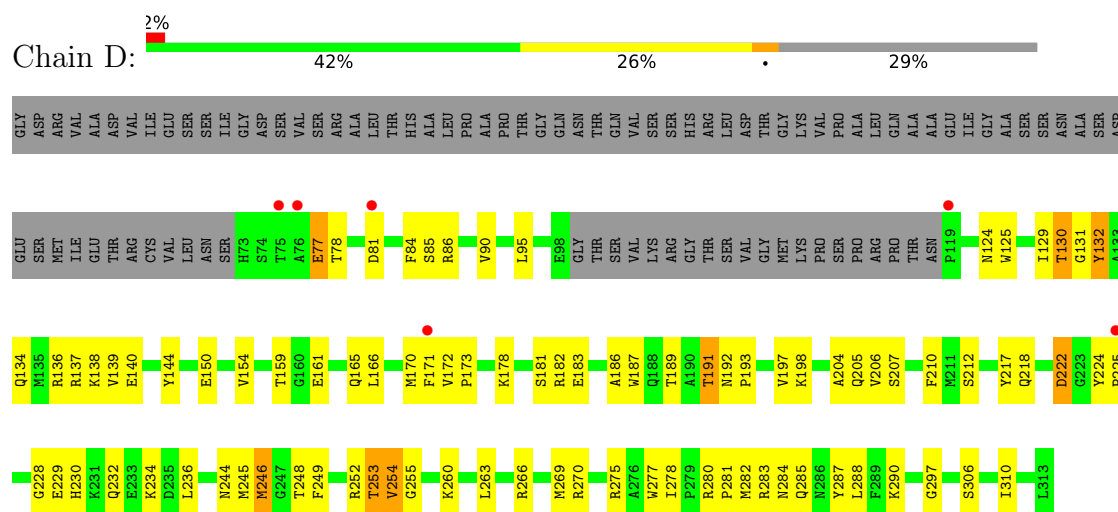
• Molecule 2: Capsid protein VP0



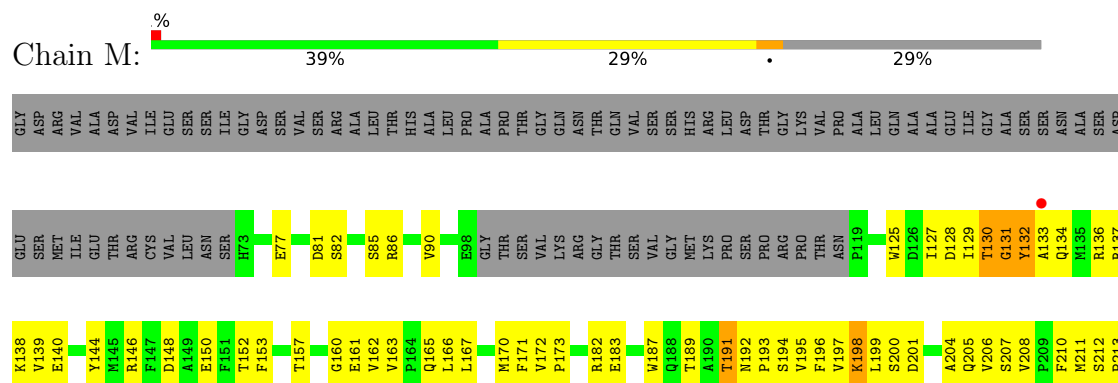
• Molecule 2: Capsid protein VP0

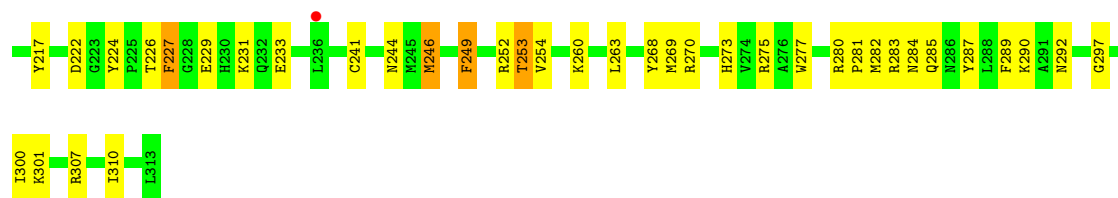


• Molecule 3: Capsid protein VP1

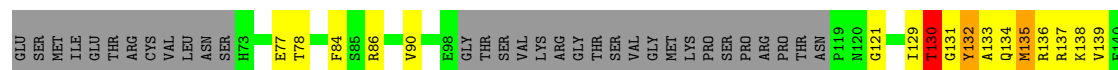
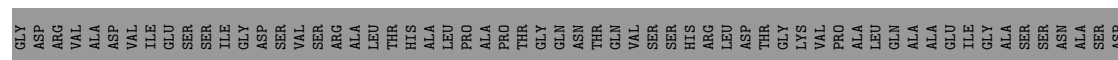
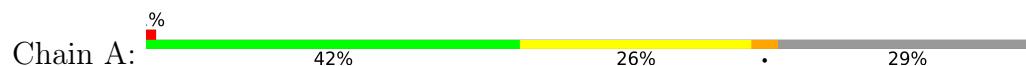


• Molecule 3: Capsid protein VP1

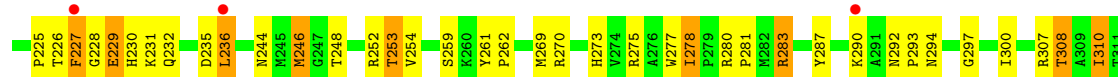
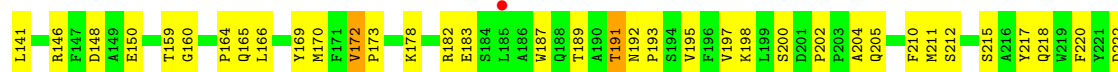
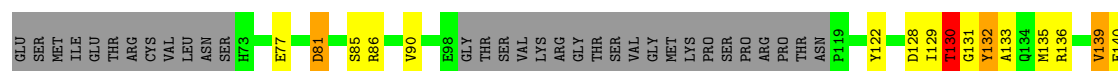




• Molecule 3: Capsid protein VP1

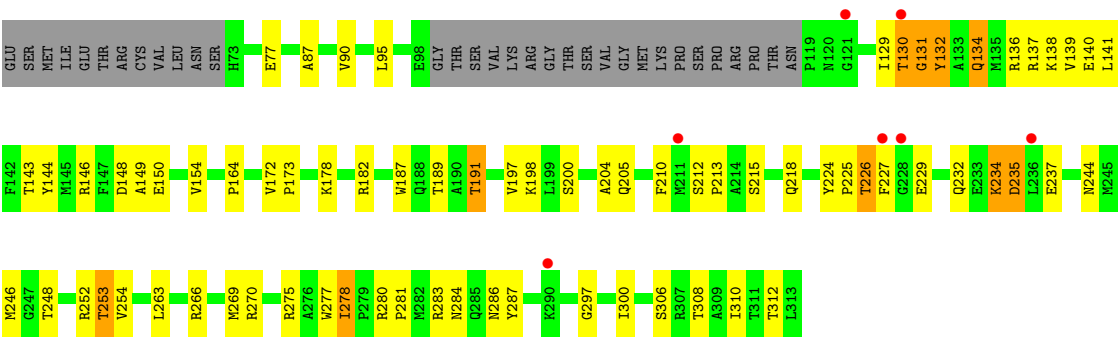


• Molecule 3: Capsid protein VP1



• Molecule 3: Capsid protein VP1





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 3 ₂	Depositor
Cell constants a, b, c, α , β , γ	350.15Å 350.15Å 350.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.79 – 3.81 46.79 – 3.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.79-3.81) 77.2 (46.79-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.271 , 0.299 0.274 , 0.303	Depositor DCC
R_{free} test set	2000 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å ²)	100.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	26425	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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	B	0.37	0/1744	0.90	7/2387 (0.3%)
1	E	0.36	0/1744	0.89	8/2387 (0.3%)
1	H	0.38	0/1744	0.94	12/2387 (0.5%)
1	K	0.35	0/1744	0.87	1/2387 (0.0%)
1	N	0.36	0/1744	0.88	6/2387 (0.3%)
2	C	0.36	0/1882	0.85	5/2580 (0.2%)
2	F	0.36	0/1882	0.85	4/2580 (0.2%)
2	I	0.39	0/1882	0.84	1/2580 (0.0%)
2	L	0.37	0/1882	0.87	4/2580 (0.2%)
2	O	0.36	0/1882	0.85	2/2580 (0.1%)
3	A	0.34	0/1811	0.85	2/2464 (0.1%)
3	D	0.35	0/1811	0.81	1/2464 (0.0%)
3	G	0.36	0/1811	0.86	4/2464 (0.2%)
3	J	0.35	0/1811	0.85	1/2464 (0.0%)
3	M	0.36	0/1811	0.84	3/2464 (0.1%)
All	All	0.36	0/27185	0.86	61/37155 (0.2%)

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	160	GLY	N-CA-C	-8.14	104.33	114.92
1	H	60	THR	N-CA-C	6.91	120.83	107.71
3	G	172	VAL	CA-C-N	6.84	127.43	120.38
3	G	172	VAL	C-N-CA	6.84	127.43	120.38
1	H	60	THR	CB-CA-C	-6.59	102.07	111.76
2	C	36	GLY	N-CA-C	-6.38	106.12	115.63
2	F	96	ALA	N-CA-C	-6.26	106.28	114.04
2	L	36	GLY	N-CA-C	-6.25	106.32	115.63
1	N	31	THR	CA-C-N	6.24	126.21	119.78
1	N	31	THR	C-N-CA	6.24	126.21	119.78
1	N	169	ILE	CA-C-N	6.18	125.40	118.97
1	N	169	ILE	C-N-CA	6.18	125.40	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	89	ASP	CA-C-N	6.18	125.91	119.05
1	H	89	ASP	C-N-CA	6.18	125.91	119.05
3	D	253	THR	N-CA-C	6.12	121.63	114.04
1	B	78	GLY	N-CA-C	6.12	118.13	110.29
3	G	160	GLY	N-CA-C	-6.12	106.97	114.92
1	H	78	GLY	N-CA-C	5.93	117.88	110.29
3	G	236	LEU	N-CA-C	-5.92	107.05	114.56
3	M	253	THR	N-CA-C	5.89	121.35	114.04
3	M	160	GLY	N-CA-C	-5.78	107.40	114.92
2	F	25	THR	CB-CA-C	-5.75	107.21	114.40
2	F	229	THR	CA-C-N	5.71	126.66	120.83
2	F	229	THR	C-N-CA	5.71	126.66	120.83
2	I	100	TYR	N-CA-C	-5.64	107.05	114.04
1	E	169	ILE	CA-C-N	5.52	124.71	118.97
1	E	169	ILE	C-N-CA	5.52	124.71	118.97
1	E	29	HIS	CA-C-N	5.48	126.25	120.11
1	E	29	HIS	C-N-CA	5.48	126.25	120.11
1	H	31	THR	CA-C-N	5.47	125.42	119.78
1	H	31	THR	C-N-CA	5.47	125.42	119.78
3	A	135	MET	N-CA-C	-5.47	105.87	112.54
1	N	89	ASP	CA-C-N	5.44	125.09	119.05
1	N	89	ASP	C-N-CA	5.44	125.09	119.05
2	L	46	ASP	N-CA-C	-5.43	103.95	111.28
1	B	36	ILE	CA-C-N	5.41	125.71	119.92
1	B	36	ILE	C-N-CA	5.41	125.71	119.92
1	B	136	THR	CA-C-N	5.41	125.95	120.38
1	B	136	THR	C-N-CA	5.41	125.95	120.38
2	C	145	HIS	CA-C-N	5.39	125.94	120.38
2	C	145	HIS	C-N-CA	5.39	125.94	120.38
3	M	198	LYS	N-CA-C	-5.39	102.91	110.35
2	L	152	GLN	CA-C-N	5.34	124.85	119.19
2	L	152	GLN	C-N-CA	5.34	124.85	119.19
1	H	169	ILE	CA-C-N	5.26	124.44	118.97
1	H	169	ILE	C-N-CA	5.26	124.44	118.97
2	O	140	GLY	N-CA-C	-5.23	107.58	114.95
1	E	226	MET	N-CA-C	-5.22	101.83	109.81
1	K	171	TRP	N-CA-C	5.21	117.00	108.76
3	J	226	THR	N-CA-C	5.16	116.57	109.15
2	O	25	THR	CB-CA-C	-5.13	107.99	114.40
1	B	75	ALA	N-CA-C	-5.12	105.78	111.36
1	H	61	ASN	N-CA-C	-5.10	96.72	111.00
2	C	195	VAL	CA-C-N	5.08	126.34	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	195	VAL	C-N-CA	5.08	126.34	120.85
1	E	9	GLY	N-CA-C	-5.07	108.08	115.63
1	B	100	LEU	N-CA-C	-5.07	105.84	111.36
1	H	142	LEU	CA-C-N	5.04	124.96	119.76
1	H	142	LEU	C-N-CA	5.04	124.96	119.76
1	E	137	PRO	CA-C-N	5.01	126.11	119.84
1	E	137	PRO	C-N-CA	5.01	126.11	119.84

There are no chirality outliers.

There are no planarity outliers.

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	B	1699	0	1691	77	0
1	E	1699	0	1691	70	0
1	H	1699	0	1691	75	0
1	K	1699	0	1691	51	0
1	N	1699	0	1691	66	0
2	C	1829	0	1765	71	0
2	F	1829	0	1765	64	0
2	I	1829	0	1765	83	0
2	L	1829	0	1765	54	0
2	O	1829	0	1765	67	0
3	A	1757	0	1707	88	0
3	D	1757	0	1707	78	0
3	G	1757	0	1707	83	0
3	J	1757	0	1707	65	0
3	M	1757	0	1707	100	0
All	All	26425	0	25815	877	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (877) 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)
2:C:12:ARG:O	2:C:26:GLN:NE2	2.10	0.84
3:J:191:THR:HG21	1:N:230:LYS:HA	1.61	0.82
3:A:136:ARG:HD3	1:B:236:LEU:HD12	1.60	0.82
1:E:121:PHE:O	2:F:184:ASN:ND2	2.13	0.81
3:A:253:THR:H	3:A:254:VAL:HA	1.44	0.81
3:A:146:ARG:NH2	1:B:33:CYS:SG	2.53	0.81
3:D:136:ARG:HH22	3:D:290:LYS:HG2	1.46	0.81
2:O:101:LEU:HG	2:O:203:PHE:HB3	1.60	0.81
1:K:121:PHE:O	2:L:184:ASN:ND2	2.14	0.80
1:B:82:LEU:HD11	1:B:85:VAL:HG13	1.62	0.80
3:M:134:GLN:NE2	1:N:232:ALA:O	2.15	0.78
2:I:12:ARG:O	2:I:26:GLN:NE2	2.15	0.78
1:E:24:ILE:HG22	1:E:25:LEU:HG	1.65	0.78
3:A:280:ARG:NH2	2:C:129:GLU:O	2.16	0.78
3:D:191:THR:HG21	1:H:230:LYS:HA	1.65	0.78
3:G:146:ARG:NH2	1:H:33:CYS:SG	2.56	0.78
1:K:138:PRO:HA	1:K:192:GLY:H	1.50	0.76
1:H:82:LEU:HD11	1:H:85:VAL:HG13	1.67	0.76
1:B:49:VAL:HG11	2:C:177:VAL:HA	1.65	0.76
3:M:90:VAL:HG21	3:M:269:MET:HB3	1.68	0.76
3:J:232:GLN:HG3	3:J:234:LYS:HB2	1.68	0.76
2:I:54:THR:N	2:I:245:PHE:O	2.20	0.75
1:E:4:THR:HG22	1:H:2:PHE:HB3	1.68	0.75
1:B:24:ILE:HG22	1:B:25:LEU:HG	1.68	0.75
3:D:205:GLN:OE1	1:H:7:LYS:NZ	2.20	0.74
1:H:71:PHE:HB2	1:H:214:ILE:HB	1.69	0.74
3:G:228:GLY:O	2:I:208:ASN:ND2	2.20	0.74
2:C:97:GLN:O	2:C:249:ARG:NH1	2.19	0.74
3:D:197:VAL:HG11	3:D:204:ALA:HB2	1.69	0.74
3:A:137:ARG:NH1	3:A:283:ARG:O	2.17	0.74
2:I:101:LEU:HG	2:I:203:PHE:HB3	1.69	0.74
3:G:308:THR:HG23	3:G:312:THR:HG21	1.70	0.74
1:N:121:PHE:O	2:O:184:ASN:ND2	2.21	0.74
1:H:121:PHE:O	2:I:184:ASN:ND2	2.19	0.73
2:F:208:ASN:ND2	3:D:228:GLY:O	2.21	0.73
1:N:24:ILE:HG22	1:N:25:LEU:HG	1.71	0.73
3:J:178:LYS:HE2	3:J:248:THR:HG21	1.70	0.73
1:E:79:LYS:HD2	1:E:80:GLY:N	2.03	0.73
2:C:101:LEU:HG	2:C:203:PHE:HB3	1.70	0.73
1:E:82:LEU:HD11	1:E:85:VAL:HG13	1.71	0.73
1:N:122:THR:HA	2:O:184:ASN:HD21	1.53	0.73
2:I:21:SER:HB2	2:I:62:ARG:HG3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:24:ILE:HG22	1:K:25:LEU:HG	1.71	0.72
2:C:25:THR:OG1	2:C:26:GLN:N	2.19	0.72
3:G:140:GLU:HG3	3:G:220:PHE:HZ	1.55	0.72
3:G:191:THR:HG21	1:B:230:LYS:HA	1.72	0.71
1:E:230:LYS:HA	3:M:191:THR:HG21	1.73	0.71
1:B:48:GLN:HE22	1:B:222:LYS:HA	1.55	0.71
1:B:121:PHE:O	2:C:184:ASN:ND2	2.23	0.71
3:M:287:TYR:HB3	1:N:237:GLN:HE22	1.54	0.71
2:O:188:ASN:ND2	2:O:190:CYS:O	2.21	0.70
3:D:218:GLN:O	3:D:244:ASN:ND2	2.23	0.70
2:C:26:GLN:HG3	2:C:27:GLU:H	1.56	0.70
3:A:191:THR:HG21	1:K:230:LYS:HA	1.72	0.70
1:E:232:ALA:O	3:D:134:GLN:NE2	2.24	0.70
3:J:253:THR:H	3:J:254:VAL:HA	1.55	0.70
3:G:197:VAL:HG11	3:G:204:ALA:HB2	1.72	0.70
3:G:218:GLN:O	3:G:244:ASN:ND2	2.24	0.70
3:M:137:ARG:NH1	3:M:283:ARG:O	2.25	0.70
3:J:197:VAL:HG11	3:J:204:ALA:HB2	1.74	0.70
3:G:280:ARG:NH2	2:I:129:GLU:O	2.25	0.70
1:K:122:THR:HA	2:L:184:ASN:HD21	1.57	0.70
2:O:187:THR:OG1	2:O:188:ASN:N	2.24	0.69
1:K:71:PHE:HB2	1:K:214:ILE:HB	1.73	0.69
1:H:122:THR:HA	2:I:184:ASN:HD21	1.57	0.69
1:E:8:PRO:O	3:M:205:GLN:NE2	2.22	0.69
3:A:197:VAL:HG11	3:A:204:ALA:HB2	1.73	0.69
2:C:31:ILE:HD12	2:C:32:ILE:H	1.58	0.69
1:B:105:CYS:HB3	1:B:111:TRP:HE1	1.58	0.69
1:N:82:LEU:HD11	1:N:85:VAL:HG13	1.75	0.68
1:H:24:ILE:HG22	1:H:25:LEU:HG	1.73	0.68
2:C:99:HIS:O	2:C:249:ARG:NH1	2.25	0.68
2:L:101:LEU:HG	2:L:203:PHE:HB3	1.75	0.68
3:D:161:GLU:OE1	3:M:260:LYS:NZ	2.26	0.68
2:C:199:ASN:ND2	2:C:204:ASP:OD2	2.27	0.68
1:H:48:GLN:HE22	1:H:222:LYS:HA	1.56	0.68
2:C:13:VAL:O	2:C:26:GLN:NE2	2.26	0.68
3:J:90:VAL:HG21	3:J:269:MET:HB3	1.76	0.68
3:M:193:PRO:HG2	1:N:24:ILE:HG23	1.76	0.68
1:K:82:LEU:HD11	1:K:85:VAL:HG13	1.76	0.68
2:L:128:PRO:HA	2:L:212:PHE:HA	1.75	0.67
2:L:187:THR:OG1	2:L:188:ASN:N	2.27	0.67
2:O:82:PHE:HE2	2:O:214:LEU:HB2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:68:THR:HG22	2:L:235:THR:HA	1.76	0.67
2:L:69:LYS:NZ	2:L:156:ASP:O	2.27	0.67
3:D:204:ALA:HA	1:H:9:GLY:HA2	1.74	0.67
3:A:283:ARG:NH1	2:C:168:ALA:O	2.28	0.67
1:K:105:CYS:HB3	1:K:111:TRP:HE1	1.59	0.67
3:A:199:LEU:O	3:G:198:LYS:NZ	2.27	0.67
2:I:188:ASN:OD1	2:I:190:CYS:N	2.27	0.67
3:M:182:ARG:NH2	3:M:253:THR:OG1	2.27	0.67
3:J:150:GLU:OE1	3:J:270:ARG:NH2	2.28	0.67
3:M:136:ARG:HH12	3:M:290:LYS:HG3	1.60	0.66
1:K:139:GLY:C	2:C:249:ARG:HE	2.02	0.66
2:F:103:ARG:NH1	2:F:244:GLU:OE1	2.27	0.66
3:J:136:ARG:NH1	3:J:140:GLU:OE2	2.27	0.66
1:B:138:PRO:HA	1:B:192:GLY:H	1.60	0.66
3:A:90:VAL:HG21	3:A:269:MET:HB3	1.75	0.66
2:I:20:ASN:N	2:I:20:ASN:OD1	2.28	0.66
3:G:205:GLN:OE1	1:H:21:SER:OG	2.12	0.66
3:G:253:THR:H	3:G:254:VAL:HA	1.60	0.66
2:F:188:ASN:ND2	2:F:190:CYS:O	2.24	0.66
3:D:186:ALA:O	3:D:192:ASN:ND2	2.28	0.66
3:G:130:THR:HG21	3:G:290:LYS:HE3	1.77	0.66
2:I:121:ALA:H	2:I:220:SER:HB3	1.60	0.66
2:F:21:SER:HB2	2:F:62:ARG:HG3	1.77	0.66
2:O:128:PRO:HA	2:O:212:PHE:HA	1.76	0.66
2:L:197:TYR:OH	2:L:204:ASP:OD2	2.10	0.66
3:A:253:THR:N	3:A:254:VAL:HA	2.08	0.65
1:B:204:VAL:HG11	1:B:210:ASN:HA	1.78	0.65
1:K:143:PRO:HB3	2:C:250:GLN:HG3	1.78	0.65
3:D:129:ILE:HG22	3:D:269:MET:HE1	1.77	0.65
2:F:187:THR:OG1	2:F:188:ASN:N	2.28	0.65
1:N:100:LEU:HD22	2:O:177:VAL:HG11	1.78	0.65
3:M:198:LYS:HG3	3:M:201:ASP:HB3	1.78	0.65
1:E:71:PHE:HB2	1:E:214:ILE:HB	1.77	0.65
3:M:82:SER:O	3:M:86:ARG:NH1	2.27	0.64
3:A:182:ARG:HH22	3:A:253:THR:HG22	1.63	0.64
3:G:170:MET:HE1	3:G:187:TRP:HA	1.79	0.64
2:I:30:ASN:ND2	2:I:181:GLN:OE1	2.30	0.64
3:A:134:GLN:NE2	1:B:231:ASP:OD2	2.30	0.64
2:C:187:THR:OG1	2:C:188:ASN:N	2.31	0.64
3:M:146:ARG:NH2	1:N:31:THR:O	2.31	0.64
2:F:57:ASP:O	2:F:61:ASN:ND2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:162:VAL:HB	3:J:164:PRO:HB2	1.80	0.63
3:A:77:GLU:OE2	1:H:29:HIS:N	2.31	0.63
3:M:253:THR:H	3:M:254:VAL:HA	1.63	0.63
3:M:229:GLU:OE2	2:O:208:ASN:ND2	2.30	0.63
3:G:210:PHE:CZ	3:G:212:SER:HB3	2.33	0.63
3:J:137:ARG:HH21	1:K:107:TYR:HE1	1.46	0.63
2:O:80:TRP:NE1	2:O:155:ALA:O	2.28	0.63
3:M:138:LYS:HG2	1:N:107:TYR:CE2	2.33	0.63
1:H:44:LEU:O	1:H:48:GLN:HG2	1.98	0.63
2:O:199:ASN:ND2	2:O:204:ASP:OD2	2.31	0.63
3:M:150:GLU:OE1	3:M:270:ARG:NH2	2.32	0.62
3:M:280:ARG:NH2	2:O:129:GLU:O	2.33	0.62
3:J:144:TYR:HB2	3:J:277:TRP:HB2	1.81	0.62
1:N:62:ALA:HA	1:N:65:LEU:HB2	1.80	0.62
1:B:85:VAL:HG12	1:B:195:SER:HA	1.80	0.62
3:G:129:ILE:HG22	3:G:269:MET:HE1	1.81	0.62
3:G:130:THR:OG1	3:G:131:GLY:N	2.32	0.62
3:J:280:ARG:NH2	2:L:129:GLU:O	2.33	0.62
2:I:12:ARG:HG3	2:I:28:ALA:HB2	1.80	0.62
3:D:253:THR:H	3:D:254:VAL:HA	1.65	0.62
1:E:48:GLN:HE22	1:E:222:LYS:HA	1.65	0.62
3:J:77:GLU:OE2	1:B:29:HIS:N	2.27	0.62
3:J:95:LEU:HB2	3:J:263:LEU:HB2	1.82	0.62
2:F:12:ARG:HD3	2:F:26:GLN:HA	1.82	0.62
1:N:130:LYS:N	1:N:200:THR:OG1	2.29	0.62
2:O:115:SER:OG	2:O:116:LYS:N	2.32	0.62
3:D:182:ARG:NH2	3:D:253:THR:OG1	2.17	0.61
3:A:121:GLY:O	3:A:182:ARG:NH1	2.33	0.61
3:M:133:ALA:HA	1:N:236:LEU:HD12	1.82	0.61
3:A:234:LYS:HE2	3:A:237:GLU:H	1.65	0.61
2:C:98:PHE:O	2:C:249:ARG:N	2.29	0.61
2:L:188:ASN:ND2	2:L:190:CYS:O	2.29	0.61
2:F:128:PRO:HA	2:F:212:PHE:HA	1.83	0.61
3:G:307:ARG:H	1:H:57:ASN:HB3	1.63	0.61
2:I:187:THR:OG1	2:I:188:ASN:N	2.31	0.61
2:L:134:THR:HG23	2:L:146:PRO:HG3	1.82	0.61
2:F:101:LEU:HG	2:F:203:PHE:HB3	1.82	0.61
3:M:307:ARG:HG3	1:N:57:ASN:HD22	1.64	0.61
1:E:122:THR:HA	2:F:184:ASN:HD21	1.66	0.61
2:O:115:SER:HB3	2:O:118:HIS:CE1	2.36	0.61
1:N:61:ASN:OD1	1:N:62:ALA:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:138:LYS:HG2	1:N:107:TYR:HE2	1.65	0.60
3:J:154:VAL:HB	3:J:266:ARG:HB2	1.83	0.60
3:D:229:GLU:HG3	3:D:230:HIS:H	1.66	0.60
3:M:241:CYS:O	3:M:244:ASN:ND2	2.30	0.60
2:C:40:SER:O	2:C:103:ARG:NH2	2.35	0.60
2:F:69:LYS:NZ	2:F:156:ASP:O	2.22	0.60
3:A:161:GLU:OE1	3:A:163:VAL:HG13	2.01	0.60
3:A:258:LYS:H	3:A:258:LYS:HD3	1.66	0.60
2:F:86:LEU:HD11	2:F:238:LEU:HD11	1.84	0.60
3:M:208:VAL:HG13	3:M:211:MET:HE3	1.83	0.59
2:I:69:LYS:NZ	2:I:156:ASP:O	2.28	0.59
1:H:204:VAL:HG11	1:H:210:ASN:HA	1.84	0.59
3:D:81:ASP:OD1	3:D:85:SER:OG	2.19	0.59
3:A:193:PRO:HG2	1:B:24:ILE:HG23	1.82	0.59
3:D:198:LYS:NZ	3:G:200:SER:O	2.36	0.59
1:K:44:LEU:O	1:K:48:GLN:HG2	2.01	0.59
1:E:24:ILE:HG23	3:D:193:PRO:HG2	1.84	0.59
3:J:150:GLU:OE2	3:J:205:GLN:NE2	2.35	0.59
1:E:55:VAL:HB	1:E:71:PHE:HE1	1.68	0.59
3:G:300:ILE:HB	1:H:62:ALA:HB2	1.84	0.59
2:L:199:ASN:ND2	2:L:204:ASP:OD2	2.35	0.59
1:E:44:LEU:O	1:E:48:GLN:HG2	2.03	0.59
3:M:81:ASP:OD1	3:M:85:SER:OG	2.19	0.59
3:A:130:THR:OG1	3:A:131:GLY:N	2.34	0.59
3:G:226:THR:HG23	3:G:227:PHE:CD1	2.37	0.59
3:G:297:GLY:HA2	3:G:300:ILE:HD11	1.85	0.59
3:J:210:PHE:CZ	3:J:212:SER:HB3	2.38	0.59
3:M:130:THR:O	3:M:132:TYR:N	2.35	0.59
1:E:8:PRO:C	3:M:205:GLN:HE21	2.10	0.58
3:J:187:TRP:CD2	3:J:252:ARG:HD2	2.37	0.58
2:F:134:THR:HG23	2:F:146:PRO:HG3	1.85	0.58
3:D:187:TRP:CD2	3:D:252:ARG:HD2	2.38	0.58
3:M:297:GLY:H	2:O:135:VAL:HG13	1.68	0.58
3:G:253:THR:N	3:G:254:VAL:HA	2.19	0.58
1:K:161:LEU:HD12	1:K:162:GLN:H	1.68	0.58
3:M:197:VAL:HG11	3:M:204:ALA:HB2	1.86	0.58
2:C:25:THR:O	2:C:26:GLN:HB2	2.03	0.58
1:H:54:GLU:OE2	2:I:164:TYR:OH	2.11	0.58
2:C:172:ILE:HD13	2:C:217:VAL:HG11	1.86	0.58
2:F:26:GLN:NE2	2:F:190:CYS:SG	2.75	0.58
3:J:297:GLY:HA3	2:L:135:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HD22	2:C:177:VAL:HG11	1.84	0.58
2:O:17:THR:HB	2:O:22:THR:HG23	1.84	0.58
2:I:23:ILE:HD13	2:I:237:THR:HG21	1.85	0.58
3:J:253:THR:N	3:J:254:VAL:HA	2.17	0.58
2:L:175:LEU:HD21	2:L:215:LEU:HD11	1.86	0.58
1:K:50:GLU:HA	1:K:219:ALA:HB2	1.86	0.58
1:E:161:LEU:HD12	1:E:162:GLN:H	1.69	0.58
3:A:297:GLY:HA2	3:A:300:ILE:HD11	1.85	0.58
3:G:90:VAL:HG21	3:G:269:MET:HB3	1.85	0.58
3:M:152:THR:N	3:M:268:TYR:O	2.33	0.57
3:D:140:GLU:OE1	3:D:287:TYR:OH	2.21	0.57
1:N:105:CYS:HB3	1:N:111:TRP:HE1	1.69	0.57
2:F:199:ASN:HD21	2:F:209:HIS:CD2	2.23	0.57
3:J:224:TYR:HD2	3:J:237:GLU:HB3	1.70	0.57
2:L:226:GLN:N	2:L:226:GLN:OE1	2.38	0.57
2:O:175:LEU:HD21	2:O:215:LEU:HD11	1.87	0.57
2:F:223:ASP:OD1	2:F:224:TYR:N	2.38	0.57
3:A:86:ARG:NH1	1:B:229:CYS:SG	2.78	0.57
1:E:46:LEU:HB3	1:E:100:LEU:HD23	1.84	0.57
1:B:55:VAL:HB	1:B:71:PHE:HE1	1.70	0.57
1:B:62:ALA:HA	1:B:65:LEU:HB2	1.85	0.57
1:E:15:THR:OG1	3:M:194:SER:N	2.37	0.57
2:C:115:SER:OG	2:C:116:LYS:N	2.38	0.57
2:F:115:SER:OG	2:F:116:LYS:N	2.37	0.57
2:F:129:GLU:O	3:D:280:ARG:NH2	2.38	0.57
3:D:130:THR:O	3:D:132:TYR:N	2.38	0.57
3:M:136:ARG:HH22	3:M:290:LYS:HG3	1.70	0.57
3:G:140:GLU:HG3	3:G:220:PHE:CZ	2.39	0.57
3:J:226:THR:HA	3:J:227:PHE:HD1	1.70	0.57
1:B:78:GLY:N	1:B:81:GLU:OE2	2.38	0.57
2:I:41:TYR:HA	2:I:103:ARG:HH12	1.69	0.57
1:H:109:THR:HG21	1:H:228:LEU:HD23	1.87	0.56
3:G:141:LEU:O	3:G:280:ARG:N	2.35	0.56
3:G:130:THR:O	3:G:132:TYR:N	2.37	0.56
2:C:223:ASP:OD1	2:C:224:TYR:N	2.39	0.56
1:E:24:ILE:HG12	3:D:206:VAL:HG11	1.87	0.56
2:I:115:SER:OG	2:I:116:LYS:N	2.36	0.56
3:A:217:TYR:OH	3:A:246:MET:SD	2.50	0.56
3:A:224:TYR:N	2:C:208:ASN:O	2.35	0.56
2:F:199:ASN:ND2	2:F:204:ASP:OD2	2.39	0.56
2:O:103:ARG:HG3	2:O:197:TYR:CG	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:TYR:HA	2:C:103:ARG:HH12	1.71	0.56
2:C:83:PRO:HD2	2:C:210:CYS:HA	1.85	0.56
2:I:23:ILE:HD11	2:I:63:PHE:CG	2.41	0.56
3:G:132:TYR:OH	1:H:231:ASP:OD2	2.23	0.56
2:O:86:LEU:HD11	2:O:238:LEU:HD11	1.87	0.56
3:G:277:TRP:NE1	1:H:36:ILE:O	2.38	0.56
2:I:249:ARG:HG2	2:I:250:GLN:H	1.71	0.56
2:F:26:GLN:NE2	2:F:189:ASN:OD1	2.39	0.56
3:J:87:ALA:HA	3:J:270:ARG:HB2	1.88	0.56
2:F:41:TYR:HA	2:F:103:ARG:HH12	1.71	0.55
3:M:129:ILE:HG22	3:M:269:MET:HE1	1.88	0.55
3:A:205:GLN:NE2	1:K:8:PRO:O	2.26	0.55
1:N:54:GLU:OE2	2:O:164:TYR:OH	2.19	0.55
2:C:30:ASN:ND2	2:C:181:GLN:OE1	2.38	0.55
2:I:249:ARG:HG2	2:I:250:GLN:N	2.21	0.55
1:N:237:GLN:H	1:N:237:GLN:CD	2.14	0.55
2:L:54:THR:N	2:L:245:PHE:O	2.40	0.55
2:L:16:LEU:O	2:L:23:ILE:N	2.39	0.55
1:K:61:ASN:OD1	1:K:62:ALA:N	2.39	0.55
2:O:40:SER:O	2:O:103:ARG:NH2	2.38	0.55
2:L:23:ILE:HD11	2:L:63:PHE:CG	2.41	0.55
2:F:103:ARG:O	2:F:244:GLU:N	2.39	0.55
1:B:50:GLU:O	2:C:176:THR:OG1	2.11	0.55
1:K:109:THR:OG1	1:K:228:LEU:HB3	2.07	0.55
1:H:62:ALA:HA	1:H:65:LEU:HB2	1.89	0.55
1:K:109:THR:OG1	1:K:110:GLN:N	2.38	0.55
1:N:56:ASN:HB3	1:N:68:ARG:HA	1.88	0.55
1:H:85:VAL:HG12	1:H:195:SER:HA	1.88	0.55
3:D:182:ARG:HH22	3:D:253:THR:HG1	1.49	0.55
3:G:290:LYS:HZ3	1:H:236:LEU:HD21	1.71	0.54
1:E:213:TYR:HD2	2:F:221:PRO:HD2	1.72	0.54
1:N:49:VAL:HG11	2:O:177:VAL:HA	1.89	0.54
3:A:162:VAL:HB	3:G:164:PRO:HB2	1.89	0.54
2:C:68:THR:HG22	2:C:235:THR:HA	1.89	0.54
1:K:130:LYS:HG2	1:K:158:ASP:HA	1.89	0.54
3:J:130:THR:O	3:J:132:TYR:N	2.41	0.54
3:J:144:TYR:HE2	2:L:198:ILE:HG22	1.73	0.54
2:I:33:VAL:HG21	2:I:181:GLN:HE21	1.71	0.54
2:F:93:GLY:O	2:F:97:GLN:HG2	2.08	0.54
3:J:138:LYS:HG2	1:K:107:TYR:CE2	2.43	0.54
2:F:16:LEU:O	2:F:23:ILE:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ASN:OD1	1:E:62:ALA:N	2.40	0.54
3:A:187:TRP:CD2	3:A:252:ARG:HD2	2.42	0.54
3:G:182:ARG:O	3:G:187:TRP:NE1	2.41	0.54
3:J:297:GLY:HA2	3:J:300:ILE:HD11	1.89	0.54
1:H:120:MET:HE1	2:I:182:TRP:CD2	2.43	0.54
3:A:198:LYS:NZ	3:J:200:SER:O	2.41	0.54
1:B:130:LYS:N	1:B:200:THR:OG1	2.30	0.54
2:I:160:LEU:HB2	2:I:167:ASP:OD2	2.08	0.54
3:D:124:ASN:HB3	3:D:178:LYS:HZ1	1.73	0.53
3:M:290:LYS:N	3:M:290:LYS:HD2	2.23	0.53
2:I:30:ASN:HD21	2:I:181:GLN:CD	2.15	0.53
2:F:135:VAL:HG13	3:D:297:GLY:H	1.74	0.53
3:M:171:PHE:O	3:M:192:ASN:HB2	2.08	0.53
3:G:146:ARG:HG3	3:G:210:PHE:CD1	2.43	0.53
3:M:253:THR:N	3:M:254:VAL:HA	2.23	0.53
1:H:100:LEU:HD22	2:I:177:VAL:HG11	1.89	0.53
1:H:105:CYS:HB3	1:H:111:TRP:HE1	1.73	0.53
3:D:136:ARG:O	3:D:140:GLU:N	2.35	0.53
3:M:182:ARG:O	3:M:187:TRP:NE1	2.42	0.53
3:J:132:TYR:O	3:J:134:GLN:N	2.37	0.53
2:F:208:ASN:O	3:D:224:TYR:N	2.32	0.53
3:D:132:TYR:OH	3:M:189:THR:O	2.15	0.53
3:G:225:PRO:O	3:G:228:GLY:N	2.41	0.53
2:F:128:PRO:HB2	3:D:278:ILE:HD13	1.91	0.53
3:M:152:THR:HG21	1:N:13:PHE:CE1	2.44	0.53
2:I:250:GLN:N	2:I:250:GLN:OE1	2.38	0.53
1:E:25:LEU:HD22	3:G:86:ARG:HH21	1.73	0.53
3:D:181:SER:OG	3:D:182:ARG:N	2.37	0.53
3:G:136:ARG:O	3:G:140:GLU:N	2.36	0.53
2:L:115:SER:OG	2:L:116:LYS:N	2.41	0.53
1:K:78:GLY:N	1:K:81:GLU:OE2	2.42	0.53
3:M:77:GLU:HG3	1:N:227:GLN:HA	1.91	0.53
3:D:253:THR:N	3:D:254:VAL:HA	2.24	0.52
3:M:140:GLU:OE1	3:M:287:TYR:OH	2.22	0.52
3:A:201:ASP:O	3:G:198:LYS:NZ	2.41	0.52
2:I:128:PRO:HA	2:I:212:PHE:HA	1.91	0.52
2:I:199:ASN:ND2	2:I:204:ASP:OD2	2.43	0.52
2:I:40:SER:O	2:I:103:ARG:NH2	2.43	0.52
3:D:234:LYS:HZ1	3:D:236:LEU:HD12	1.74	0.52
3:J:237:GLU:N	3:J:237:GLU:OE1	2.41	0.52
1:E:120:MET:HE1	2:F:182:TRP:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:144:TYR:HB2	3:D:277:TRP:HB2	1.91	0.52
3:J:146:ARG:NE	3:J:215:SER:O	2.35	0.52
1:N:46:LEU:HB3	1:N:100:LEU:HD23	1.89	0.52
1:E:12:GLN:HA	3:M:197:VAL:HG12	1.92	0.52
1:K:125:PHE:HB3	2:L:116:LYS:HB3	1.90	0.52
2:C:69:LYS:NZ	2:C:156:ASP:O	2.28	0.52
3:A:133:ALA:C	3:A:136:ARG:HE	2.17	0.52
3:A:169:TYR:HB2	3:A:195:VAL:HB	1.91	0.52
1:H:105:CYS:HB3	1:H:111:TRP:NE1	2.24	0.52
2:C:82:PHE:HE2	2:C:214:LEU:HB2	1.75	0.52
3:A:169:TYR:O	3:A:195:VAL:N	2.37	0.52
1:B:61:ASN:OD1	1:B:62:ALA:N	2.43	0.52
1:E:204:VAL:HG11	1:E:210:ASN:HA	1.92	0.52
3:J:130:THR:OG1	3:J:131:GLY:N	2.42	0.52
2:I:184:ASN:O	2:I:188:ASN:N	2.42	0.52
1:E:107:TYR:CE1	3:D:282:MET:HE1	2.45	0.51
3:A:134:GLN:O	3:A:138:LYS:HG3	2.10	0.51
3:G:193:PRO:HG2	1:H:24:ILE:HG23	1.92	0.51
1:E:21:SER:OG	1:H:7:LYS:NZ	2.34	0.51
3:A:306:SER:OG	1:B:68:ARG:NH2	2.43	0.51
1:K:55:VAL:HB	1:K:71:PHE:HE1	1.75	0.51
2:O:223:ASP:OD1	2:O:224:TYR:N	2.42	0.51
1:E:227:GLN:NE2	1:N:29:HIS:O	2.44	0.51
3:A:77:GLU:O	1:B:108:TYR:OH	2.16	0.51
3:G:292:ASN:OD1	3:G:294:ASN:ND2	2.24	0.51
3:G:297:GLY:HA3	2:I:135:VAL:HG13	1.93	0.51
1:B:46:LEU:HB3	1:B:100:LEU:HD23	1.92	0.51
2:O:16:LEU:O	2:O:23:ILE:N	2.40	0.51
1:B:109:THR:OG1	1:B:110:GLN:N	2.44	0.51
1:E:31:THR:OG1	3:D:212:SER:O	2.20	0.51
1:E:107:TYR:OH	3:D:137:ARG:NE	2.44	0.51
2:F:165:VAL:HG12	3:D:284:ASN:HD21	1.75	0.51
1:N:130:LYS:HG2	1:N:158:ASP:HA	1.93	0.51
2:C:188:ASN:ND2	2:C:190:CYS:O	2.40	0.51
3:J:275:ARG:HH21	1:K:39:GLU:CD	2.19	0.50
2:O:250:GLN:OE1	2:O:250:GLN:N	2.39	0.50
1:E:14:LEU:HG	1:E:16:THR:H	1.76	0.50
3:D:165:GLN:OE1	3:D:166:LEU:N	2.41	0.50
3:M:282:MET:HE1	1:N:107:TYR:CE1	2.46	0.50
1:N:14:LEU:HG	1:N:16:THR:H	1.76	0.50
1:K:109:THR:HG22	1:K:230:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:23:ILE:HG22	2:O:24:THR:H	1.77	0.50
2:C:175:LEU:HD21	2:C:215:LEU:HD11	1.93	0.50
1:E:109:THR:OG1	1:E:110:GLN:N	2.43	0.50
3:D:90:VAL:HG21	3:D:269:MET:HB3	1.93	0.50
3:M:157:THR:HG1	3:M:161:GLU:N	2.09	0.50
1:N:109:THR:OG1	1:N:110:GLN:N	2.44	0.50
1:B:91:GLY:HA3	1:B:111:TRP:CZ2	2.46	0.50
2:F:250:GLN:OE1	2:F:250:GLN:N	2.40	0.50
3:A:290:LYS:HE2	1:B:236:LEU:HD11	1.93	0.50
3:J:148:ASP:OD1	3:J:149:ALA:N	2.44	0.50
3:M:152:THR:HG23	3:M:205:GLN:HB3	1.93	0.50
1:H:130:LYS:N	1:H:200:THR:OG1	2.38	0.50
2:L:119:GLN:O	2:L:222:LEU:HA	2.11	0.50
1:E:109:THR:OG1	1:E:228:LEU:HB3	2.12	0.50
3:M:217:TYR:OH	3:M:246:MET:SD	2.52	0.50
3:A:138:LYS:HG2	1:B:107:TYR:CE2	2.46	0.50
3:J:278:ILE:HD13	2:L:128:PRO:HG2	1.93	0.50
1:H:61:ASN:OD1	1:H:62:ALA:N	2.45	0.50
2:I:80:TRP:NE1	2:I:155:ALA:O	2.42	0.50
2:L:66:LEU:HD12	2:L:236:ILE:HG21	1.93	0.50
3:D:95:LEU:HB2	3:D:263:LEU:HB2	1.92	0.50
3:M:163:VAL:H	3:M:199:LEU:HD11	1.77	0.50
3:J:146:ARG:NH2	1:K:31:THR:O	2.45	0.50
1:N:85:VAL:HG12	1:N:195:SER:HA	1.91	0.50
1:E:57:ASN:HB3	3:D:306:SER:HB3	1.93	0.50
3:M:297:GLY:HA2	3:M:300:ILE:HD11	1.93	0.50
1:N:109:THR:HG22	1:N:230:LYS:HD3	1.93	0.50
1:H:118:THR:N	1:H:217:LEU:O	2.39	0.50
2:O:70:LEU:HD13	2:O:231:VAL:HG11	1.93	0.50
3:D:234:LYS:NZ	3:D:236:LEU:HB2	2.27	0.50
3:J:129:ILE:HG22	3:J:269:MET:HE1	1.93	0.50
1:N:138:PRO:HA	1:N:192:GLY:H	1.77	0.50
1:B:115:LEU:HB2	1:B:169:ILE:HB	1.94	0.50
2:C:199:ASN:HB3	2:C:201:LEU:O	2.12	0.49
2:I:57:ASP:O	2:I:61:ASN:ND2	2.45	0.49
3:D:183:GLU:OE1	3:D:183:GLU:N	2.45	0.49
3:A:310:ILE:HD12	1:B:84:ALA:HB2	1.92	0.49
1:K:146:ARG:HD2	1:K:199:GLN:OE1	2.12	0.49
2:I:12:ARG:HB2	2:I:26:GLN:HG3	1.93	0.49
1:E:122:THR:HA	2:F:184:ASN:ND2	2.28	0.49
3:D:217:TYR:OH	3:D:246:MET:SD	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:THR:HG22	1:K:2:PHE:HB3	1.94	0.49
2:F:21:SER:OG	2:F:63:PHE:HB2	2.12	0.49
3:A:152:THR:HG23	3:A:205:GLN:HB3	1.95	0.49
3:A:234:LYS:HD2	3:A:235:ASP:N	2.28	0.49
2:I:115:SER:HB3	2:I:118:HIS:ND1	2.27	0.49
3:M:144:TYR:HB2	3:M:277:TRP:HB2	1.94	0.49
3:A:130:THR:O	3:A:132:TYR:N	2.45	0.49
3:J:136:ARG:HB3	3:J:287:TYR:HE2	1.77	0.49
3:A:182:ARG:O	3:A:187:TRP:NE1	2.46	0.49
1:B:44:LEU:O	1:B:48:GLN:HG2	2.11	0.49
1:K:85:VAL:HG12	1:K:195:SER:HA	1.92	0.49
2:I:250:GLN:H	2:I:250:GLN:CD	2.20	0.49
3:D:225:PRO:O	3:D:228:GLY:N	2.45	0.49
3:M:170:MET:HE1	3:M:187:TRP:HA	1.93	0.49
3:J:218:GLN:O	3:J:244:ASN:ND2	2.46	0.49
1:H:74:SER:HB3	1:H:211:THR:HG23	1.95	0.49
3:J:189:THR:C	3:J:191:THR:H	2.20	0.49
1:N:55:VAL:HB	1:N:71:PHE:HE1	1.78	0.49
1:H:55:VAL:HB	1:H:71:PHE:HE1	1.78	0.49
3:A:242:PRO:O	3:A:245:MET:HG2	2.13	0.49
3:G:129:ILE:HD12	3:G:139:VAL:HG21	1.94	0.49
1:N:109:THR:HG21	1:N:228:LEU:HD23	1.94	0.49
1:H:109:THR:OG1	1:H:110:GLN:N	2.45	0.49
1:E:13:PHE:HB3	3:M:196:PHE:HB2	1.95	0.49
3:M:189:THR:HG23	3:M:192:ASN:OD1	2.13	0.49
3:M:275:ARG:HH21	1:N:39:GLU:CD	2.21	0.49
2:O:250:GLN:H	2:O:250:GLN:CD	2.20	0.49
1:E:227:GLN:HA	3:D:77:GLU:OE1	2.12	0.48
3:J:197:VAL:HG12	1:N:12:GLN:HA	1.95	0.48
2:O:68:THR:HG22	2:O:235:THR:HA	1.94	0.48
1:E:91:GLY:HA3	1:E:111:TRP:CZ2	2.49	0.48
3:M:146:ARG:NH1	1:N:33:CYS:SG	2.81	0.48
3:G:165:GLN:OE1	3:G:166:LEU:N	2.37	0.48
2:F:17:THR:HB	2:F:22:THR:HG23	1.95	0.48
3:G:132:TYR:CD2	3:G:135:MET:HE2	2.49	0.48
3:G:150:GLU:OE1	1:H:21:SER:OG	2.31	0.48
3:G:205:GLN:NE2	1:B:8:PRO:HG2	2.29	0.48
3:J:284:ASN:HD21	2:L:165:VAL:HG12	1.78	0.48
3:D:86:ARG:NH1	3:M:191:THR:OG1	2.45	0.48
3:G:283:ARG:NH2	3:G:293:PRO:O	2.46	0.48
1:E:24:ILE:HG12	3:D:206:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:224:TYR:O	2:O:208:ASN:HB3	2.13	0.48
1:K:118:THR:N	1:K:217:LEU:O	2.37	0.48
1:E:118:THR:N	1:E:217:LEU:O	2.46	0.48
3:J:234:LYS:O	3:J:235:ASP:HB2	2.13	0.48
1:B:6:LEU:H	1:H:10:THR:HB	1.79	0.48
1:H:221:GLN:HG3	1:H:222:LYS:H	1.79	0.48
3:M:153:PHE:HZ	3:M:249:PHE:CE2	2.31	0.48
3:G:226:THR:HA	3:G:227:PHE:HD1	1.79	0.48
1:H:91:GLY:HA3	1:H:111:TRP:CZ2	2.49	0.48
2:C:70:LEU:HD13	2:C:231:VAL:HG11	1.96	0.48
2:C:128:PRO:HA	2:C:212:PHE:HA	1.95	0.48
2:L:107:CYS:N	2:L:239:ALA:O	2.39	0.48
2:L:223:ASP:OD1	2:L:224:TYR:N	2.46	0.48
2:I:152:GLN:HG2	2:I:210:CYS:SG	2.54	0.48
3:D:150:GLU:HG2	3:D:270:ARG:HB3	1.94	0.47
3:A:129:ILE:HG22	3:A:269:MET:HE1	1.96	0.47
1:B:71:PHE:HB2	1:B:214:ILE:HB	1.95	0.47
1:B:146:ARG:HD2	1:B:199:GLN:OE1	2.14	0.47
3:M:290:LYS:HE2	1:N:236:LEU:HD22	1.96	0.47
3:A:144:TYR:HB2	3:A:277:TRP:HB2	1.96	0.47
1:B:132:LEU:HB3	1:B:197:TRP:HB2	1.95	0.47
1:K:51:THR:HG21	1:K:100:LEU:HB2	1.97	0.47
2:O:39:PRO:HB3	2:O:196:PRO:HA	1.96	0.47
3:D:150:GLU:HA	3:D:207:SER:HA	1.96	0.47
3:A:292:ASN:CG	3:A:294:ASN:HD22	2.18	0.47
3:J:284:ASN:HB3	2:L:171:PRO:HD3	1.96	0.47
3:D:154:VAL:HB	3:D:266:ARG:HB2	1.97	0.47
3:A:232:GLN:C	3:A:234:LYS:H	2.23	0.47
2:I:107:CYS:N	2:I:239:ALA:O	2.41	0.47
1:E:39:GLU:CD	3:D:275:ARG:HH21	2.22	0.47
3:M:167:LEU:HD21	3:M:263:LEU:HD13	1.96	0.47
3:A:136:ARG:HH12	1:B:235:ILE:C	2.22	0.47
3:G:178:LYS:HE3	3:G:248:THR:HG21	1.97	0.47
1:B:131:MET:HG3	1:B:159:PHE:CZ	2.50	0.47
2:I:17:THR:HB	2:I:22:THR:HG23	1.97	0.47
1:E:109:THR:HG22	1:E:230:LYS:HD3	1.96	0.47
2:F:94:GLN:C	2:F:96:ALA:H	2.21	0.47
1:B:35:HIS:CD2	1:B:35:HIS:C	2.92	0.47
2:C:100:TYR:HE2	2:C:247:GLY:HA3	1.80	0.47
2:L:250:GLN:N	2:L:250:GLN:OE1	2.45	0.47
1:E:105:CYS:HB3	1:E:111:TRP:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:183:GLU:N	3:M:183:GLU:OE1	2.48	0.47
3:M:222:ASP:OD1	2:O:81:LYS:NZ	2.45	0.47
3:J:182:ARG:HH22	3:J:253:THR:HG22	1.80	0.47
2:F:85:VAL:HG13	2:F:155:ALA:HA	1.96	0.47
3:A:159:THR:HG23	3:G:259:SER:HA	1.96	0.47
3:A:234:LYS:HD2	3:A:236:LEU:H	1.80	0.47
3:G:281:PRO:HB3	2:I:174:GLN:HB2	1.96	0.47
1:N:91:GLY:HA3	1:N:111:TRP:CZ2	2.50	0.47
1:N:120:MET:HE1	2:O:182:TRP:CD2	2.50	0.47
1:B:48:GLN:NE2	1:B:222:LYS:HA	2.26	0.47
1:B:132:LEU:HD13	1:B:146:ARG:HG3	1.95	0.47
2:L:146:PRO:HA	2:L:147:PRO:HD3	1.82	0.47
2:F:115:SER:HB3	2:F:118:HIS:ND1	2.30	0.47
3:D:159:THR:HG21	3:M:260:LYS:HZ2	1.79	0.47
3:A:146:ARG:HH22	1:B:33:CYS:HG	1.57	0.47
3:A:226:THR:HA	3:A:227:PHE:HA	1.52	0.47
3:G:222:ASP:OD1	2:I:81:LYS:NZ	2.35	0.47
3:J:224:TYR:HA	3:J:225:PRO:HD3	1.83	0.47
3:J:286:ASN:ND2	1:K:235:ILE:HD11	2.30	0.47
1:E:127:ALA:O	2:F:186:ARG:NH2	2.48	0.46
3:G:290:LYS:HZ3	1:H:236:LEU:HD11	1.81	0.46
2:I:223:ASP:OD1	2:I:224:TYR:N	2.47	0.46
1:E:131:MET:HA	1:E:199:GLN:H	1.80	0.46
1:E:169:ILE:HG21	1:E:172:ILE:HD11	1.98	0.46
2:F:115:SER:HB3	2:F:118:HIS:CE1	2.49	0.46
3:D:210:PHE:CZ	3:D:212:SER:HB3	2.50	0.46
3:A:210:PHE:CZ	3:A:212:SER:HB3	2.49	0.46
1:B:120:MET:HE1	2:C:182:TRP:CD2	2.50	0.46
2:I:30:ASN:HD22	2:I:188:ASN:ND2	2.12	0.46
1:E:163:SER:OG	2:F:186:ARG:HD3	2.16	0.46
2:F:82:PHE:CE1	2:F:238:LEU:HD22	2.50	0.46
3:M:226:THR:HA	3:M:227:PHE:HA	1.68	0.46
3:M:284:ASN:HB3	2:O:171:PRO:HG3	1.98	0.46
3:A:136:ARG:NH1	1:B:236:LEU:HB2	2.31	0.46
3:J:137:ARG:NH1	3:J:283:ARG:O	2.48	0.46
2:O:82:PHE:CE1	2:O:238:LEU:HD22	2.51	0.46
3:G:290:LYS:NZ	1:H:236:LEU:HD11	2.29	0.46
3:J:141:LEU:O	3:J:280:ARG:N	2.44	0.46
2:O:81:LYS:HD2	2:O:151:THR:O	2.16	0.46
2:O:103:ARG:O	2:O:244:GLU:N	2.48	0.46
2:C:26:GLN:HG3	2:C:27:GLU:N	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:73:LYS:HG3	2:I:222:LEU:O	2.16	0.46
2:O:98:PHE:HA	2:O:249:ARG:HG2	1.96	0.46
2:I:188:ASN:OD1	2:I:188:ASN:C	2.58	0.46
3:G:281:PRO:HG2	2:I:170:ILE:CG2	2.46	0.46
1:B:54:GLU:OE2	2:C:164:TYR:OH	2.19	0.46
2:O:82:PHE:HE1	2:O:238:LEU:HD22	1.80	0.46
1:E:130:LYS:N	1:E:200:THR:OG1	2.27	0.46
1:B:74:SER:OG	1:B:76:GLN:HG2	2.16	0.46
2:O:72:GLU:H	2:O:72:GLU:HG2	1.56	0.46
3:G:275:ARG:HH21	1:H:39:GLU:CD	2.22	0.46
2:O:123:LEU:N	2:O:217:VAL:O	2.48	0.46
2:I:82:PHE:HE1	2:I:238:LEU:HD22	1.80	0.46
1:N:71:PHE:HB2	1:N:214:ILE:HB	1.98	0.46
1:H:47:CYS:HB3	1:H:101:LEU:HD13	1.97	0.46
2:O:103:ARG:HG3	2:O:197:TYR:CD1	2.50	0.46
2:O:197:TYR:OH	2:O:204:ASP:OD2	2.31	0.46
3:M:136:ARG:HD2	1:N:236:LEU:HD21	1.98	0.45
3:A:172:VAL:HB	3:A:248:THR:OG1	2.15	0.45
3:A:282:MET:HE1	1:B:107:TYR:CE1	2.51	0.45
2:I:80:TRP:HB3	2:I:85:VAL:HG22	1.96	0.45
2:L:164:TYR:O	2:L:171:PRO:HA	2.16	0.45
3:D:254:VAL:HG12	3:D:255:GLY:H	1.80	0.45
3:M:136:ARG:NH1	3:M:290:LYS:HG3	2.30	0.45
3:J:226:THR:CA	3:J:227:PHE:HD1	2.29	0.45
2:C:54:THR:N	2:C:245:PHE:O	2.49	0.45
2:F:102:TYR:OH	2:F:104:SER:OG	2.26	0.45
1:N:60:THR:HA	1:N:61:ASN:HA	1.79	0.45
2:C:17:THR:HG23	2:C:22:THR:OG1	2.16	0.45
2:I:12:ARG:HE	2:I:28:ALA:HA	1.81	0.45
2:L:80:TRP:HB3	2:L:85:VAL:CG2	2.47	0.45
3:D:283:ARG:NH1	3:D:285:GLN:O	2.49	0.45
3:G:81:ASP:O	3:G:85:SER:HB3	2.16	0.45
1:N:150:MET:O	1:N:154:HIS:ND1	2.49	0.45
2:O:94:GLN:C	2:O:96:ALA:H	2.25	0.45
1:E:73:VAL:HA	1:E:198:TYR:OH	2.17	0.45
2:F:79:TYR:HA	2:F:215:LEU:HA	1.98	0.45
3:D:132:TYR:O	3:D:134:GLN:N	2.40	0.45
3:D:170:MET:HE1	3:D:187:TRP:HA	1.99	0.45
3:D:234:LYS:NZ	3:D:236:LEU:HD12	2.31	0.45
3:M:134:GLN:O	3:M:138:LYS:HG3	2.16	0.45
3:G:133:ALA:HB1	1:H:236:LEU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:THR:O	2:I:119:GLN:HB2	2.17	0.45
1:H:146:ARG:HA	1:H:149:ALA:HB3	1.97	0.45
2:I:182:TRP:O	2:I:188:ASN:ND2	2.49	0.45
1:E:8:PRO:HG2	3:M:205:GLN:NE2	2.31	0.45
3:M:195:VAL:HG21	3:M:206:VAL:HG21	1.98	0.45
3:G:187:TRP:CD2	3:G:252:ARG:HD3	2.51	0.45
1:N:122:THR:O	2:O:119:GLN:HB2	2.16	0.45
1:B:54:GLU:HB2	1:B:98:SER:HB3	1.98	0.45
1:H:163:SER:OG	2:I:186:ARG:HD3	2.17	0.45
2:O:31:ILE:HG13	2:O:32:ILE:H	1.80	0.45
2:C:99:HIS:HA	2:C:248:LEU:HA	1.99	0.45
2:C:103:ARG:NH1	2:C:244:GLU:OE1	2.49	0.45
2:C:103:ARG:O	2:C:244:GLU:N	2.50	0.45
2:L:80:TRP:HB3	2:L:85:VAL:HG21	1.98	0.45
3:G:183:GLU:N	3:G:183:GLU:OE1	2.50	0.45
3:J:77:GLU:HG3	1:K:227:GLN:HA	1.99	0.45
2:I:19:GLY:C	2:I:20:ASN:OD1	2.60	0.45
2:F:100:TYR:HE2	2:F:247:GLY:HA3	1.81	0.45
2:F:152:GLN:HG2	2:F:210:CYS:SG	2.56	0.45
3:A:141:LEU:O	3:A:280:ARG:N	2.43	0.45
1:B:2:PHE:HA	1:B:3:PRO:HD3	1.78	0.45
2:L:204:ASP:CG	2:L:209:HIS:HD2	2.24	0.45
1:E:22:ALA:HA	1:E:23:PRO:HD3	1.85	0.45
3:G:202:PRO:HB3	1:H:11:ASN:HD22	1.82	0.45
3:J:308:THR:OG1	3:J:312:THR:HG21	2.17	0.45
1:H:108:TYR:HA	1:H:228:LEU:O	2.17	0.45
3:A:135:MET:SD	3:A:271:MET:HE3	2.57	0.44
3:A:275:ARG:HH21	1:B:39:GLU:CD	2.25	0.44
1:N:76:GLN:HA	1:N:77:ALA:C	2.41	0.44
1:N:140:GLY:HA3	2:L:249:ARG:HD2	1.99	0.44
1:B:201:ASN:OD1	1:B:202:TYR:N	2.47	0.44
1:H:132:LEU:HD13	1:H:146:ARG:HG3	1.99	0.44
1:K:52:ILE:HB	2:L:173:SER:HA	1.99	0.44
1:K:138:PRO:O	1:K:190:THR:OG1	2.25	0.44
2:O:100:TYR:CZ	2:O:101:LEU:HD13	2.52	0.44
2:C:115:SER:HB3	2:C:118:HIS:CE1	2.51	0.44
3:G:150:GLU:OE2	3:G:270:ARG:NH2	2.42	0.44
3:G:217:TYR:OH	3:G:246:MET:SD	2.59	0.44
1:N:78:GLY:N	1:N:81:GLU:OE2	2.41	0.44
1:N:150:MET:HE2	1:N:150:MET:HB3	1.92	0.44
1:H:131:MET:HG3	1:H:159:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:ALA:HA	1:E:65:LEU:HB2	1.99	0.44
3:G:252:ARG:NH2	3:G:254:VAL:HB	2.32	0.44
3:J:77:GLU:OE1	1:B:28:PHE:HA	2.17	0.44
3:G:229:GLU:HB3	3:G:230:HIS:H	1.61	0.44
2:C:73:LYS:HG3	2:C:222:LEU:O	2.18	0.44
2:L:101:LEU:HD12	2:L:101:LEU:HA	1.82	0.44
2:F:126:VAL:HG22	2:F:214:LEU:HD23	2.00	0.44
2:F:249:ARG:HD2	1:H:140:GLY:HA3	1.98	0.44
3:A:224:TYR:HA	3:A:225:PRO:HD3	1.83	0.44
1:B:122:THR:HA	2:C:184:ASN:HD21	1.81	0.44
1:H:109:THR:HG22	1:H:230:LYS:HD3	2.00	0.44
2:O:188:ASN:CG	2:O:190:CYS:H	2.25	0.44
1:B:74:SER:OG	1:B:76:GLN:O	2.35	0.44
1:H:74:SER:HA	1:H:211:THR:HA	2.00	0.44
1:K:22:ALA:HA	1:K:23:PRO:HD3	1.79	0.44
1:K:161:LEU:HD12	1:K:162:GLN:N	2.31	0.44
2:O:80:TRP:HB3	2:O:85:VAL:HG22	1.99	0.44
2:C:15:GLN:C	2:C:16:LEU:HD23	2.43	0.44
1:E:238:THR:O	3:D:290:LYS:NZ	2.46	0.44
2:F:239:ALA:HA	2:F:240:PRO:HD3	1.84	0.44
3:D:124:ASN:HB3	3:D:178:LYS:NZ	2.31	0.44
3:M:187:TRP:CD2	3:M:252:ARG:HD2	2.53	0.44
3:A:78:THR:OG1	1:B:42:ASN:ND2	2.48	0.44
1:N:89:ASP:HA	1:N:90:PRO:HD3	1.86	0.44
2:I:176:THR:HG22	2:I:180:HIS:CD2	2.53	0.44
1:E:55:VAL:HB	1:E:71:PHE:CE1	2.50	0.44
1:B:98:SER:HB2	2:C:173:SER:HB3	2.00	0.44
1:K:48:GLN:HE22	1:K:222:LYS:HA	1.83	0.44
2:O:57:ASP:O	2:O:61:ASN:ND2	2.50	0.44
3:M:171:PHE:HB2	3:M:249:PHE:HE1	1.83	0.44
3:A:227:PHE:CG	3:A:228:GLY:N	2.86	0.44
1:N:146:ARG:HD2	1:N:199:GLN:OE1	2.17	0.44
2:I:94:GLN:C	2:I:96:ALA:H	2.26	0.44
1:E:6:LEU:HD21	1:H:6:LEU:HD13	2.00	0.43
3:M:132:TYR:OH	3:J:189:THR:O	2.23	0.43
3:G:169:TYR:HB2	3:G:195:VAL:HB	1.98	0.43
3:J:283:ARG:HD2	2:L:169:GLY:O	2.18	0.43
1:K:140:GLY:HA3	2:C:249:ARG:HD3	2.00	0.43
2:C:21:SER:OG	2:C:63:PHE:HB2	2.18	0.43
2:C:23:ILE:HD11	2:C:63:PHE:CG	2.53	0.43
2:C:148:TYR:HD2	2:C:149:LYS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:THR:HG1	1:E:102:GLY:H	1.60	0.43
2:F:71:TRP:CZ3	2:F:122:LEU:HD11	2.53	0.43
3:A:136:ARG:NH1	1:B:234:ASP:OD2	2.51	0.43
3:A:136:ARG:HG3	3:A:137:ARG:H	1.82	0.43
3:J:224:TYR:N	2:L:208:ASN:O	2.46	0.43
1:B:145:ASP:O	1:B:148:THR:OG1	2.32	0.43
2:I:82:PHE:HE2	2:I:214:LEU:HB2	1.83	0.43
3:M:148:ASP:OD2	3:M:273:HIS:ND1	2.51	0.43
1:B:213:TYR:HD2	2:C:221:PRO:HD2	1.83	0.43
2:O:115:SER:HB3	2:O:118:HIS:ND1	2.33	0.43
1:E:60:THR:HA	1:E:61:ASN:HA	1.74	0.43
3:A:288:LEU:HD23	3:A:288:LEU:HA	1.88	0.43
3:J:306:SER:HB3	1:K:57:ASN:HB3	2.01	0.43
1:N:146:ARG:NH1	1:N:146:ARG:HB3	2.33	0.43
1:B:118:THR:N	1:B:217:LEU:O	2.46	0.43
1:B:150:MET:HE2	1:B:150:MET:HB3	1.96	0.43
2:C:145:HIS:HA	2:C:146:PRO:HD3	1.85	0.43
2:I:175:LEU:HD21	2:I:215:LEU:HD11	2.00	0.43
2:I:197:TYR:OH	2:I:204:ASP:OD2	2.18	0.43
3:M:128:ASP:N	3:M:128:ASP:OD1	2.52	0.43
3:M:289:PHE:HB2	3:M:292:ASN:OD1	2.18	0.43
3:G:132:TYR:HD2	3:G:135:MET:HE2	1.82	0.43
1:B:109:THR:HG21	1:B:228:LEU:HD23	2.00	0.43
1:K:60:THR:HA	1:K:61:ASN:HA	1.74	0.43
2:C:163:PRO:C	2:C:172:ILE:HD11	2.44	0.43
2:I:82:PHE:CE1	2:I:238:LEU:HD22	2.54	0.43
3:D:232:GLN:HG2	3:D:234:LYS:O	2.18	0.43
1:N:22:ALA:HA	1:N:23:PRO:HD3	1.82	0.43
1:H:212:ALA:HA	2:I:119:GLN:HE22	1.84	0.43
2:I:101:LEU:HD12	2:I:101:LEU:HA	1.78	0.43
1:E:132:LEU:HD21	1:E:134:ALA:HB2	2.01	0.43
3:M:77:GLU:OE1	3:M:77:GLU:N	2.41	0.43
3:M:307:ARG:H	1:N:57:ASN:HB3	1.84	0.43
3:G:292:ASN:CG	3:G:294:ASN:HD22	2.19	0.43
3:J:281:PRO:HG2	2:L:170:ILE:CG2	2.49	0.43
1:H:146:ARG:HD2	1:H:199:GLN:OE1	2.18	0.43
2:O:249:ARG:HG3	2:O:250:GLN:N	2.34	0.43
3:A:254:VAL:HG23	3:A:255:GLY:O	2.18	0.43
1:B:73:VAL:HA	1:B:198:TYR:OH	2.19	0.43
1:H:131:MET:HE2	1:H:159:PHE:CZ	2.53	0.43
1:K:146:ARG:NH1	1:K:146:ARG:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:23:ILE:HD11	2:F:63:PHE:CD1	2.53	0.43
3:D:260:LYS:HE3	3:G:159:THR:HG21	2.01	0.43
3:M:229:GLU:CD	2:O:208:ASN:HD21	2.24	0.43
3:G:128:ASP:OD1	3:G:128:ASP:N	2.51	0.43
3:G:172:VAL:HA	3:G:173:PRO:HD2	1.76	0.43
1:N:143:PRO:HD3	2:L:250:GLN:HE21	1.83	0.43
1:N:158:ASP:OD1	1:N:161:LEU:HG	2.19	0.43
1:H:134:ALA:HA	1:H:154:HIS:HA	2.01	0.43
1:K:122:THR:O	2:L:119:GLN:HB2	2.19	0.43
1:E:29:HIS:HA	1:E:30:PRO:HD3	1.86	0.42
3:A:183:GLU:OE1	3:A:183:GLU:N	2.51	0.42
3:A:290:LYS:HA	3:A:290:LYS:HD3	1.67	0.42
3:A:292:ASN:OD1	3:A:294:ASN:ND2	2.26	0.42
3:J:213:PRO:HG3	1:N:110:GLN:NE2	2.34	0.42
1:K:82:LEU:HD23	1:K:197:TRP:CE2	2.53	0.42
2:O:101:LEU:HD12	2:O:101:LEU:HA	1.63	0.42
2:I:133:GLY:N	2:I:167:ASP:O	2.47	0.42
1:E:24:ILE:CG2	3:D:193:PRO:HG2	2.48	0.42
3:M:210:PHE:CZ	3:M:212:SER:HB3	2.53	0.42
3:A:132:TYR:OH	3:A:134:GLN:NE2	2.45	0.42
3:G:261:TYR:HA	3:G:262:PRO:HD3	1.83	0.42
2:O:199:ASN:HB3	2:O:201:LEU:O	2.20	0.42
2:L:17:THR:HB	2:L:22:THR:HG23	2.01	0.42
3:M:132:TYR:O	3:M:134:GLN:N	2.48	0.42
3:A:136:ARG:NH1	1:B:235:ILE:O	2.49	0.42
3:A:205:GLN:NE2	1:K:8:PRO:HG2	2.34	0.42
3:G:136:ARG:CZ	3:G:287:TYR:HE2	2.32	0.42
3:G:215:SER:OG	1:H:34:ILE:HG12	2.19	0.42
3:G:307:ARG:NH1	3:G:310:ILE:HA	2.34	0.42
1:H:48:GLN:NE2	1:H:222:LYS:HA	2.28	0.42
1:K:67:GLU:HG2	1:K:70:ARG:NH2	2.34	0.42
2:F:30:ASN:ND2	2:F:181:GLN:OE1	2.53	0.42
3:G:236:LEU:HD12	2:I:145:HIS:CE1	2.55	0.42
3:G:278:ILE:HD13	2:I:128:PRO:HB2	2.01	0.42
1:B:60:THR:HA	1:B:61:ASN:HA	1.70	0.42
1:H:123:GLY:O	2:I:186:ARG:HB2	2.19	0.42
2:C:250:GLN:N	2:C:250:GLN:CD	2.78	0.42
2:I:93:GLY:O	2:I:97:GLN:HG2	2.19	0.42
2:I:163:PRO:C	2:I:172:ILE:HD11	2.45	0.42
3:A:170:MET:HE1	3:A:187:TRP:HA	2.02	0.42
3:A:281:PRO:HG2	2:C:170:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:172:VAL:HA	3:J:173:PRO:HD2	1.85	0.42
1:E:146:ARG:HB3	1:E:146:ARG:NH1	2.35	0.42
2:F:146:PRO:HA	2:F:147:PRO:HD3	1.74	0.42
3:M:125:TRP:CZ3	3:M:127:ILE:HA	2.55	0.42
3:M:157:THR:OG1	3:M:161:GLU:N	2.53	0.42
3:M:198:LYS:HD2	3:M:200:SER:OG	2.20	0.42
3:A:284:ASN:HD21	2:C:165:VAL:HG12	1.85	0.42
1:B:75:ALA:HA	1:B:202:TYR:HB3	2.01	0.42
2:O:21:SER:OG	2:O:63:PHE:HB2	2.20	0.42
2:I:81:LYS:O	2:I:84:ASP:HB3	2.20	0.42
3:D:288:LEU:HD23	3:D:288:LEU:HA	1.84	0.42
3:A:283:ARG:HD2	2:C:169:GLY:O	2.20	0.42
2:L:17:THR:HA	2:L:22:THR:HA	2.00	0.42
2:L:239:ALA:HA	2:L:240:PRO:HD3	1.87	0.42
1:E:54:GLU:OE2	2:F:164:TYR:OH	2.16	0.42
2:F:70:LEU:HD13	2:F:231:VAL:HG11	2.01	0.42
2:F:185:LEU:H	2:F:185:LEU:HD12	1.85	0.42
3:D:172:VAL:HB	3:D:248:THR:OG1	2.19	0.42
3:M:212:SER:HA	3:M:213:PRO:HD3	1.94	0.42
3:M:281:PRO:HG2	2:O:170:ILE:CG2	2.50	0.42
3:A:145:MET:O	3:A:217:TYR:N	2.51	0.42
3:A:147:PHE:HB3	3:A:274:VAL:HG12	2.02	0.42
3:A:189:THR:C	3:A:191:THR:H	2.27	0.42
3:J:281:PRO:HG2	2:L:170:ILE:HG21	2.02	0.42
1:H:93:SER:HA	1:H:94:GLY:HA3	1.53	0.42
2:O:23:ILE:HD11	2:O:63:PHE:CD1	2.55	0.42
2:I:164:TYR:O	2:I:171:PRO:HA	2.20	0.42
3:M:130:THR:OG1	3:M:131:GLY:N	2.53	0.42
3:M:282:MET:HG3	1:N:100:LEU:HD11	2.01	0.42
3:G:277:TRP:NE1	1:H:39:GLU:HB2	2.34	0.42
2:C:110:VAL:O	2:C:191:ALA:N	2.50	0.42
1:E:228:LEU:HD21	3:M:173:PRO:HB2	2.02	0.42
3:M:200:SER:O	3:J:198:LYS:NZ	2.50	0.42
3:A:232:GLN:O	3:A:233:GLU:HB3	2.19	0.42
1:K:158:ASP:OD1	1:K:161:LEU:HG	2.20	0.42
2:O:107:CYS:HB2	2:O:241:MET:SD	2.60	0.42
2:I:84:ASP:OD2	2:I:154:GLY:N	2.48	0.42
2:F:71:TRP:HB3	2:F:232:ILE:O	2.20	0.41
3:D:90:VAL:HG12	3:D:125:TRP:HZ2	1.85	0.41
1:B:67:GLU:HG2	1:B:70:ARG:CZ	2.50	0.41
1:H:114:SER:OG	1:H:170:PRO:O	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:GLY:HA2	1:H:141:PRO:HD3	1.89	0.41
1:K:145:ASP:O	1:K:148:THR:OG1	2.30	0.41
1:K:221:GLN:HG3	1:K:222:LYS:H	1.85	0.41
2:I:119:GLN:O	2:I:222:LEU:HA	2.20	0.41
2:L:152:GLN:HG2	2:L:210:CYS:SG	2.60	0.41
1:E:16:THR:HG21	3:M:193:PRO:HG3	2.01	0.41
1:E:42:ASN:ND2	3:D:78:THR:OG1	2.53	0.41
2:F:23:ILE:HG22	2:F:24:THR:H	1.84	0.41
3:D:173:PRO:HB2	1:H:228:LEU:HD21	2.01	0.41
1:H:130:LYS:O	1:H:199:GLN:HB3	2.20	0.41
1:K:124:SER:O	2:L:186:ARG:NH2	2.53	0.41
2:C:18:ILE:O	2:C:20:ASN:N	2.53	0.41
2:C:162:HIS:HA	2:C:163:PRO:HD2	1.95	0.41
2:I:111:GLN:O	2:I:235:THR:N	2.52	0.41
3:D:84:PHE:HE1	3:D:138:LYS:HG2	1.85	0.41
3:M:285:GLN:HA	3:M:301:LYS:HE3	2.02	0.41
3:J:136:ARG:NE	3:J:287:TYR:CE2	2.88	0.41
1:H:122:THR:HA	2:I:184:ASN:ND2	2.29	0.41
2:O:152:GLN:HG2	2:O:210:CYS:SG	2.61	0.41
2:O:164:TYR:O	2:O:171:PRO:HA	2.20	0.41
2:O:239:ALA:HA	2:O:240:PRO:HD3	1.92	0.41
2:I:81:LYS:HD2	2:I:151:THR:O	2.20	0.41
1:E:124:SER:OG	1:E:125:PHE:N	2.53	0.41
3:M:192:ASN:OD1	3:M:192:ASN:N	2.52	0.41
3:G:77:GLU:OE1	1:H:227:GLN:HA	2.21	0.41
3:G:189:THR:HG23	3:G:192:ASN:OD1	2.19	0.41
3:J:189:THR:O	3:J:191:THR:N	2.52	0.41
1:B:122:THR:OG1	1:B:213:TYR:O	2.22	0.41
2:C:106:PHE:N	2:C:195:VAL:O	2.46	0.41
2:I:23:ILE:HG22	2:I:24:THR:H	1.85	0.41
2:I:104:SER:OG	2:I:105:GLY:N	2.52	0.41
3:M:144:TYR:OH	2:O:129:GLU:OE2	2.37	0.41
3:M:281:PRO:HB3	2:O:174:GLN:HB2	2.02	0.41
3:A:306:SER:HB3	1:B:57:ASN:HB3	2.02	0.41
3:G:128:ASP:HB2	3:G:130:THR:HG22	2.02	0.41
3:G:277:TRP:HB3	3:G:278:ILE:H	1.63	0.41
1:B:22:ALA:HA	1:B:23:PRO:HD3	1.74	0.41
1:B:122:THR:O	2:C:119:GLN:HB2	2.21	0.41
3:A:84:PHE:O	3:A:86:ARG:N	2.49	0.41
3:A:172:VAL:HA	3:A:173:PRO:HD2	1.82	0.41
1:N:7:LYS:HE2	1:N:7:LYS:HB3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:82:PHE:CE1	2:C:238:LEU:HD22	2.54	0.41
2:L:86:LEU:HD11	2:L:238:LEU:HD11	2.02	0.41
1:E:21:SER:OG	3:D:205:GLN:OE1	2.39	0.41
3:A:137:ARG:NH2	1:B:103:GLN:OE1	2.54	0.41
1:N:204:VAL:O	1:N:205:PRO:C	2.63	0.41
3:M:172:VAL:HA	3:M:173:PRO:HD2	1.86	0.41
1:N:146:ARG:HA	1:N:149:ALA:HB3	2.02	0.41
1:E:133:ILE:HG22	1:E:167:LEU:HD22	2.02	0.41
2:F:68:THR:HG22	2:F:235:THR:HA	2.02	0.41
3:D:171:PHE:HD2	3:D:249:PHE:CE1	2.39	0.41
3:D:189:THR:HG23	3:D:192:ASN:OD1	2.20	0.41
3:M:150:GLU:HA	3:M:207:SER:HA	2.02	0.41
3:M:165:GLN:OE1	3:M:166:LEU:N	2.46	0.41
3:M:282:MET:HE2	3:M:282:MET:HB3	1.92	0.41
3:G:211:MET:HE2	3:G:211:MET:HB3	1.97	0.41
3:J:143:THR:HB	3:J:278:ILE:HG13	2.03	0.41
1:N:36:ILE:HA	1:N:37:PRO:HD3	1.95	0.41
1:N:54:GLU:HG3	1:N:98:SER:HB3	2.03	0.41
2:F:23:ILE:HD11	2:F:63:PHE:CG	2.55	0.41
3:A:249:PHE:HD1	3:A:249:PHE:HA	1.77	0.41
1:N:14:LEU:HD23	1:N:17:ASP:HB3	2.03	0.41
2:C:23:ILE:HD11	2:C:63:PHE:CD1	2.55	0.41
2:I:44:ASP:OD1	2:I:44:ASP:N	2.53	0.41
1:E:227:GLN:HA	3:D:77:GLU:CD	2.47	0.40
2:F:174:GLN:HB2	3:D:281:PRO:HB3	2.02	0.40
3:A:282:MET:HE2	3:A:282:MET:HB3	1.89	0.40
3:A:297:GLY:H	2:C:135:VAL:HG13	1.86	0.40
3:G:148:ASP:CG	3:G:273:HIS:HD1	2.29	0.40
1:E:52:ILE:HB	2:F:173:SER:HA	2.03	0.40
2:F:107:CYS:HB2	2:F:241:MET:HE3	2.02	0.40
3:D:187:TRP:CG	3:D:252:ARG:HD2	2.56	0.40
3:A:86:ARG:HH21	3:A:138:LYS:NZ	2.20	0.40
1:N:142:LEU:HA	1:N:143:PRO:HD2	1.94	0.40
1:H:100:LEU:HD12	1:H:100:LEU:HA	1.95	0.40
2:O:102:TYR:OH	2:O:104:SER:OG	2.24	0.40
2:C:100:TYR:CD1	2:C:101:LEU:HD13	2.55	0.40
3:M:173:PRO:HD2	3:M:192:ASN:HB3	2.04	0.40
1:B:14:LEU:HG	1:B:16:THR:H	1.87	0.40
1:B:114:SER:HB2	1:B:221:GLN:CB	2.50	0.40
2:I:14:ALA:HB2	2:I:26:GLN:NE2	2.37	0.40
2:I:109:HIS:N	2:I:237:THR:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:188:ASN:OD1	2:I:189:ASN:N	2.54	0.40
2:L:23:ILE:HG22	2:L:24:THR:H	1.86	0.40
2:L:103:ARG:HD2	2:L:202:PRO:O	2.21	0.40
1:H:130:LYS:HG2	1:H:158:ASP:HA	2.03	0.40
1:H:204:VAL:O	1:H:205:PRO:C	2.63	0.40
2:C:103:ARG:HG3	2:C:197:TYR:CG	2.56	0.40
2:L:81:LYS:O	2:L:85:VAL:HG23	2.21	0.40
2:F:81:LYS:HD3	3:D:222:ASP:OD2	2.22	0.40
3:D:189:THR:C	3:D:191:THR:H	2.28	0.40
3:M:285:GLN:NE2	2:O:165:VAL:HG11	2.37	0.40
3:G:133:ALA:HA	1:H:236:LEU:HD13	2.03	0.40
1:K:49:VAL:HG11	2:L:177:VAL:HA	2.03	0.40
2:O:33:VAL:HG21	2:O:181:GLN:HG2	2.04	0.40
2:I:103:ARG:HG3	2:I:197:TYR:CG	2.56	0.40
2:L:249:ARG:HG3	2:L:250:GLN:O	2.22	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	B	219/242 (90%)	193 (88%)	23 (10%)	3 (1%)	9	37
1	E	219/242 (90%)	192 (88%)	25 (11%)	2 (1%)	14	45
1	H	219/242 (90%)	191 (87%)	26 (12%)	2 (1%)	14	45
1	K	219/242 (90%)	193 (88%)	24 (11%)	2 (1%)	14	45
1	N	219/242 (90%)	194 (89%)	22 (10%)	3 (1%)	9	37
2	C	232/323 (72%)	195 (84%)	30 (13%)	7 (3%)	3	25
2	F	232/323 (72%)	200 (86%)	29 (12%)	3 (1%)	9	38
2	I	232/323 (72%)	201 (87%)	26 (11%)	5 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	232/323 (72%)	203 (88%)	24 (10%)	5 (2%)	5	30
2	O	232/323 (72%)	201 (87%)	26 (11%)	5 (2%)	5	30
3	A	217/313 (69%)	192 (88%)	20 (9%)	5 (2%)	5	30
3	D	217/313 (69%)	193 (89%)	20 (9%)	4 (2%)	6	33
3	G	217/313 (69%)	192 (88%)	20 (9%)	5 (2%)	5	30
3	J	217/313 (69%)	189 (87%)	22 (10%)	6 (3%)	4	26
3	M	217/313 (69%)	188 (87%)	24 (11%)	5 (2%)	5	30
All	All	3340/4390 (76%)	2917 (87%)	361 (11%)	62 (2%)	6	32

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	205	PRO
2	F	211	ASN
3	D	130	THR
3	M	130	THR
3	J	234	LYS
3	J	235	ASP
1	N	205	PRO
1	B	205	PRO
1	H	205	PRO
1	K	205	PRO
2	O	211	ASN
2	C	13	VAL
2	C	26	GLN
2	C	211	ASN
2	I	211	ASN
2	L	211	ASN
2	F	19	GLY
3	A	130	THR
3	A	231	LYS
3	A	232	GLN
3	G	130	THR
3	G	231	LYS
3	G	232	GLN
3	J	130	THR
1	H	94	GLY
2	O	31	ILE
2	C	19	GLY
2	I	19	GLY

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Mol	Chain	Res	Type
2	I	31	ILE
2	L	19	GLY
3	M	231	LYS
3	G	235	ASP
2	C	12	ARG
2	C	14	ALA
2	I	140	GLY
2	I	229	THR
3	M	132	TYR
3	M	233	GLU
3	G	132	TYR
1	N	11	ASN
1	N	94	GLY
1	B	94	GLY
1	K	94	GLY
2	O	95	ASN
2	L	229	THR
1	E	94	GLY
3	D	222	ASP
3	A	132	TYR
3	J	132	TYR
3	J	229	GLU
1	B	11	ASN
2	O	229	THR
2	C	229	THR
2	L	61	ASN
2	L	95	ASN
2	F	229	THR
3	D	132	TYR
3	A	222	ASP
3	D	131	GLY
2	O	19	GLY
3	M	131	GLY
3	J	131	GLY

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	B	187/202 (93%)	179 (96%)	8 (4%)	26	50
1	E	187/202 (93%)	180 (96%)	7 (4%)	30	54
1	H	187/202 (93%)	178 (95%)	9 (5%)	23	47
1	K	187/202 (93%)	182 (97%)	5 (3%)	39	59
1	N	187/202 (93%)	180 (96%)	7 (4%)	30	54
2	C	200/272 (74%)	193 (96%)	7 (4%)	32	54
2	F	200/272 (74%)	195 (98%)	5 (2%)	42	61
2	I	200/272 (74%)	192 (96%)	8 (4%)	28	52
2	L	200/272 (74%)	195 (98%)	5 (2%)	42	61
2	O	200/272 (74%)	189 (94%)	11 (6%)	19	45
3	A	190/265 (72%)	180 (95%)	10 (5%)	20	45
3	D	190/265 (72%)	183 (96%)	7 (4%)	30	54
3	G	190/265 (72%)	177 (93%)	13 (7%)	14	40
3	J	190/265 (72%)	183 (96%)	7 (4%)	30	54
3	M	190/265 (72%)	184 (97%)	6 (3%)	34	56
All	All	2885/3695 (78%)	2770 (96%)	115 (4%)	28	52

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	20	VAL
1	E	24	ILE
1	E	33	CYS
1	E	70	ARG
1	E	82	LEU
1	E	161	LEU
1	E	235	ILE
2	F	23	ILE
2	F	101	LEU
2	F	141	THR
2	F	238	LEU
2	F	248	LEU
3	D	77	GLU
3	D	139	VAL
3	D	191	THR
3	D	245	MET
3	D	246	MET
3	D	254	VAL

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Mol	Chain	Res	Type
3	D	310	ILE
3	M	139	VAL
3	M	191	THR
3	M	227	PHE
3	M	246	MET
3	M	249	PHE
3	M	310	ILE
3	A	130	THR
3	A	139	VAL
3	A	163	VAL
3	A	191	THR
3	A	206	VAL
3	A	246	MET
3	A	249	PHE
3	A	253	THR
3	A	258	LYS
3	A	278	ILE
3	G	81	ASP
3	G	122	TYR
3	G	130	THR
3	G	139	VAL
3	G	191	THR
3	G	227	PHE
3	G	229	GLU
3	G	246	MET
3	G	253	THR
3	G	278	ILE
3	G	283	ARG
3	G	308	THR
3	G	310	ILE
3	J	134	GLN
3	J	139	VAL
3	J	191	THR
3	J	246	MET
3	J	253	THR
3	J	278	ILE
3	J	310	ILE
1	N	7	LYS
1	N	20	VAL
1	N	24	ILE
1	N	33	CYS
1	N	70	ARG

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Mol	Chain	Res	Type
1	N	82	LEU
1	N	161	LEU
1	B	10	THR
1	B	20	VAL
1	B	33	CYS
1	B	35	HIS
1	B	70	ARG
1	B	79	LYS
1	B	82	LEU
1	B	235	ILE
1	H	20	VAL
1	H	24	ILE
1	H	33	CYS
1	H	60	THR
1	H	70	ARG
1	H	79	LYS
1	H	82	LEU
1	H	92	ARG
1	H	97	GLN
1	K	20	VAL
1	K	33	CYS
1	K	82	LEU
1	K	161	LEU
1	K	235	ILE
2	O	18	ILE
2	O	23	ILE
2	O	31	ILE
2	O	72	GLU
2	O	76	LYS
2	O	95	ASN
2	O	100	TYR
2	O	101	LEU
2	O	142	GLU
2	O	238	LEU
2	O	248	LEU
2	C	23	ILE
2	C	31	ILE
2	C	62	ARG
2	C	101	LEU
2	C	141	THR
2	C	181	GLN
2	C	238	LEU

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Mol	Chain	Res	Type
2	I	13	VAL
2	I	20	ASN
2	I	23	ILE
2	I	101	LEU
2	I	104	SER
2	I	113	ASN
2	I	180	HIS
2	I	252	VAL
2	L	23	ILE
2	L	101	LEU
2	L	181	GLN
2	L	238	LEU
2	L	248	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	35	HIS
1	E	76	GLN
1	E	174	ASN
2	F	26	GLN
2	F	30	ASN
2	F	199	ASN
3	D	243	ASN
3	D	284	ASN
3	M	205	GLN
3	M	218	GLN
3	M	243	ASN
3	A	243	ASN
3	A	244	ASN
3	J	124	ASN
3	J	243	ASN
1	N	35	HIS
1	N	76	GLN
1	N	110	GLN
1	N	237	GLN
1	B	29	HIS
1	B	35	HIS
1	B	110	GLN
1	B	221	GLN
1	K	48	GLN
2	O	97	GLN

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Mol	Chain	Res	Type
2	O	180	HIS
2	O	181	GLN
2	C	30	ASN
2	C	162	HIS
2	C	209	HIS
2	I	30	ASN
2	I	97	GLN
2	I	119	GLN
2	I	145	HIS
2	I	161	GLN
2	I	181	GLN
2	L	26	GLN
2	L	145	HIS
2	L	181	GLN
2	L	209	HIS

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	B	223/242 (92%)	0.31	4 (1%) 67 46	80, 97, 139, 197	0
1	E	223/242 (92%)	0.34	5 (2%) 62 44	80, 95, 135, 176	0
1	H	223/242 (92%)	0.52	13 (5%) 29 23	80, 96, 135, 178	0
1	K	223/242 (92%)	0.32	8 (3%) 46 32	80, 97, 140, 188	0
1	N	223/242 (92%)	0.35	3 (1%) 75 53	80, 97, 134, 201	0
2	C	236/323 (73%)	0.32	7 (2%) 52 36	78, 105, 203, 251	0
2	F	236/323 (73%)	0.36	5 (2%) 63 44	78, 103, 198, 239	0
2	I	236/323 (73%)	0.54	16 (6%) 23 20	78, 105, 205, 239	0
2	L	236/323 (73%)	0.43	8 (3%) 48 33	78, 107, 203, 235	0
2	O	236/323 (73%)	0.37	10 (4%) 40 29	78, 105, 205, 234	0
3	A	221/313 (70%)	0.20	3 (1%) 73 51	75, 95, 166, 239	0
3	D	221/313 (70%)	0.25	6 (2%) 56 38	75, 93, 164, 211	0
3	G	221/313 (70%)	0.27	4 (1%) 67 46	75, 95, 167, 237	0
3	J	221/313 (70%)	0.18	7 (3%) 50 35	75, 95, 170, 255	0
3	M	221/313 (70%)	0.18	2 (0%) 81 60	75, 95, 159, 219	0
All	All	3400/4390 (77%)	0.33	101 (2%) 52 36	75, 97, 184, 255	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	251	ALA	6.3
2	C	47	ALA	6.2
2	I	47	ALA	6.0
1	E	236	LEU	4.5
1	B	236	LEU	4.5
2	O	250	GLN	4.2
2	O	47	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	I	120	GLY	4.0
1	H	45	GLU	4.0
1	E	1	GLY	3.9
3	G	290	LYS	3.8
1	H	236	LEU	3.8
2	C	135	VAL	3.4
3	M	133	ALA	3.3
2	L	230	PRO	3.3
2	L	100	TYR	3.3
1	N	167	LEU	3.2
2	C	251	ALA	3.2
2	I	251	ALA	3.1
1	H	227	GLN	3.0
1	H	161	LEU	3.0
3	D	119	PRO	2.9
1	K	236	LEU	2.9
2	L	251	ALA	2.9
1	B	174	ASN	2.9
1	B	88	ALA	2.9
1	E	201	ASN	2.9
3	G	236	LEU	2.8
1	E	80	GLY	2.8
1	K	161	LEU	2.8
3	D	81	ASP	2.7
2	I	14	ALA	2.7
2	F	32	ILE	2.7
1	H	168	VAL	2.7
3	G	227	PHE	2.7
2	I	20	ASN	2.6
2	O	29	ALA	2.6
2	L	47	ALA	2.6
1	K	1	GLY	2.6
3	J	130	THR	2.6
1	E	87	ARG	2.6
1	H	110	GLN	2.6
2	O	32	ILE	2.5
3	J	236	LEU	2.5
2	O	58	VAL	2.5
1	N	201	ASN	2.5
3	J	227	PHE	2.5
2	I	146	PRO	2.5
2	I	145	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	171	PHE	2.5
2	I	37	GLU	2.5
1	K	27	ASN	2.5
1	K	201	ASN	2.5
1	H	151	LEU	2.5
2	F	23	ILE	2.5
2	O	60	VAL	2.5
2	I	132	ILE	2.4
2	L	247	GLY	2.4
3	D	75	THR	2.4
2	I	252	VAL	2.4
2	L	32	ILE	2.4
2	L	80	TRP	2.4
2	O	24	THR	2.4
2	C	225	ASP	2.4
2	C	212	PHE	2.3
2	I	106	PHE	2.3
1	H	61	ASN	2.3
1	H	201	ASN	2.3
3	G	185	LEU	2.3
2	F	251	ALA	2.3
2	O	14	ALA	2.3
2	L	135	VAL	2.2
1	K	166	THR	2.2
1	N	72	PRO	2.2
2	O	31	ILE	2.2
2	C	246	ALA	2.1
3	D	76	ALA	2.1
3	M	236	LEU	2.2
3	J	211	MET	2.2
1	H	152	GLY	2.1
2	C	145	HIS	2.1
3	D	225	PRO	2.1
3	J	121	GLY	2.1
1	K	174	ASN	2.1
3	J	290	LYS	2.1
2	I	125	ALA	2.1
3	A	286	ASN	2.1
3	A	282	MET	2.1
1	H	89	ASP	2.1
3	J	228	GLY	2.1
2	I	62	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	86	PHE	2.1
2	I	214	LEU	2.1
1	K	202	TYR	2.0
1	H	230	LYS	2.0
2	F	231	VAL	2.0
1	B	95	PRO	2.0
3	A	236	LEU	2.0
2	F	47	ALA	2.0
2	I	243	SER	2.0
2	I	246	ALA	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.