



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 07:50 AM EDT

PDB ID : 3NVM / pdb_00003nvm
Title : Structural basis for substrate placement by an archaeal box C/D ribonucleo-
protein particle
Authors : Xue, S.; Wang, R.; Li, H.
Deposited on : 2010-07-08
Resolution : 3.41 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

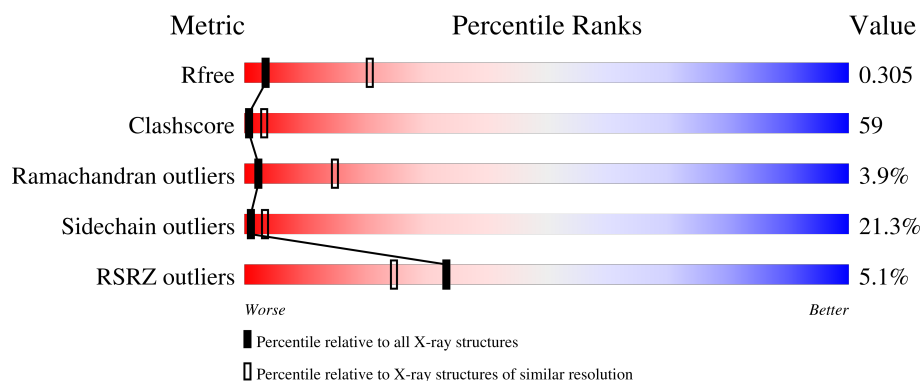
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	371	5% 31% 44% 15% 8%
2	B	234	4% 28% 49% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4597 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 NOP5/NOP56 related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2775	1770	479	519	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q8U4M1
A	-4	HIS	-	expression tag	UNP Q8U4M1
A	-3	HIS	-	expression tag	UNP Q8U4M1
A	-2	HIS	-	expression tag	UNP Q8U4M1
A	-1	HIS	-	expression tag	UNP Q8U4M1
A	0	HIS	-	expression tag	UNP Q8U4M1
A	1	HIS	-	expression tag	UNP Q8U4M1
A	2	VAL	-	expression tag	UNP Q8U4M1
A	3	MET	-	expression tag	UNP Q8U4M1
A	4	ILE	-	expression tag	UNP Q8U4M1
A	?	-	VAL	deletion	UNP Q8U4M1
A	?	-	ASP	deletion	UNP Q8U4M1
A	?	-	LYS	deletion	UNP Q8U4M1
A	?	-	VAL	deletion	UNP Q8U4M1
A	?	-	ASP	deletion	UNP Q8U4M1
A	?	-	ARG	deletion	UNP Q8U4M1
A	?	-	LEU	deletion	UNP Q8U4M1
A	?	-	TYR	deletion	UNP Q8U4M1

- Molecule 2 is a protein called Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1822	1174	312	334	2			

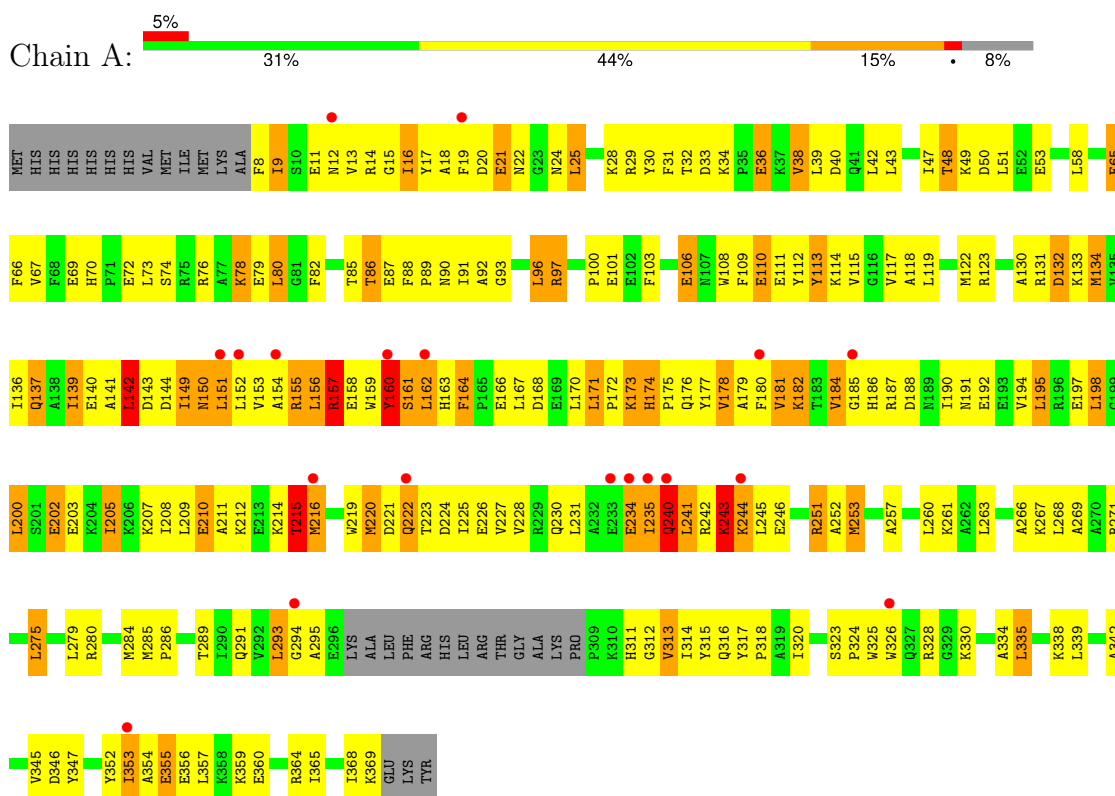
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	expression tag	UNP Q8U4M2
B	-5	HIS	-	expression tag	UNP Q8U4M2
B	-4	HIS	-	expression tag	UNP Q8U4M2
B	-3	HIS	-	expression tag	UNP Q8U4M2
B	-2	HIS	-	expression tag	UNP Q8U4M2
B	-1	HIS	-	expression tag	UNP Q8U4M2
B	0	HIS	-	expression tag	UNP Q8U4M2

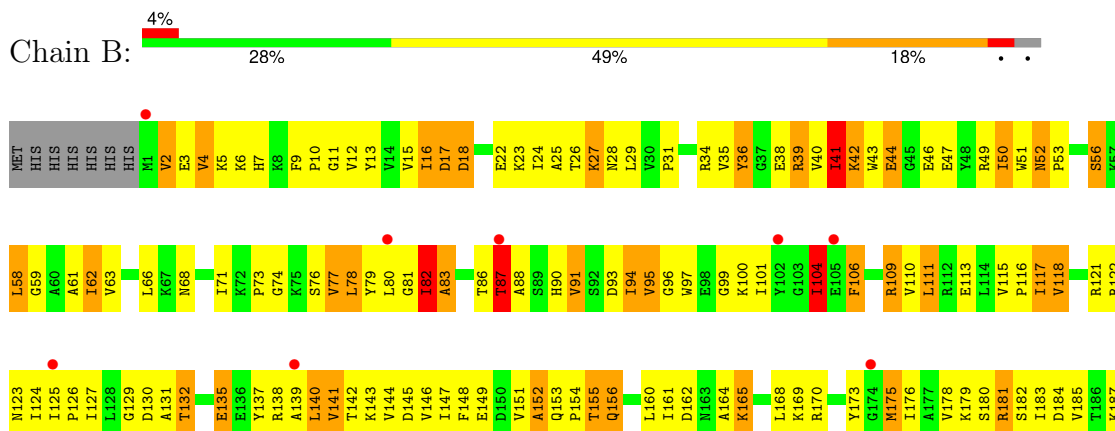
3 Residue-property plots [i](#)

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: NOP5/NOP56 related protein



• Molecule 2: Fibrillar-like rRNA/tRNA 2'-O-methyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	100.62Å 100.62Å 265.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.43 – 3.41 49.43 – 3.41	Depositor EDS
% Data completeness (in resolution range)	76.7 (49.43-3.41) 83.2 (49.43-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.242 , 0.316 0.244 , 0.305	Depositor DCC
R_{free} test set	907 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	126.8	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 224.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.063 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4597	wwPDB-VP
Average B, all atoms (Å ²)	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/2824	0.93	7/3800 (0.2%)
2	B	0.56	0/1861	1.01	8/2515 (0.3%)
All	All	0.54	0/4685	0.96	15/6315 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	52	ASN	CA-C-N	5.74	125.44	119.64
2	B	52	ASN	C-N-CA	5.74	125.44	119.64
2	B	104	ILE	N-CA-C	5.71	121.22	109.34
2	B	82	ILE	N-CA-C	5.69	121.17	109.34
2	B	94	ILE	CB-CA-C	-5.59	104.71	112.04
1	A	240	GLN	N-CA-C	5.55	117.41	111.36
2	B	132	THR	N-CA-C	-5.44	105.78	112.90
1	A	9	ILE	N-CA-C	5.43	116.54	108.23
1	A	80	LEU	N-CA-C	-5.29	107.20	113.97
1	A	132	ASP	N-CA-C	-5.22	105.71	111.71
2	B	210	LEU	N-CA-C	5.09	117.02	108.73
2	B	4	VAL	N-CA-C	5.07	115.28	107.77
1	A	164	PHE	CA-C-N	5.07	124.57	119.19
1	A	164	PHE	C-N-CA	5.07	124.57	119.19
1	A	353	ILE	N-CA-C	-5.03	106.55	111.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2775	0	2805	321	0
2	B	1822	0	1869	242	0
All	All	4597	0	4674	545	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 59.

All (545) 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:B:109:ARG:HH11	2:B:109:ARG:HG2	0.98	1.08
2:B:4:VAL:HG23	2:B:15:VAL:HG12	1.46	0.97
2:B:43:TRP:HD1	2:B:44:GLU:HG3	1.30	0.96
1:A:173:LYS:O	1:A:176:GLN:HG2	1.63	0.95
1:A:167:LEU:HD23	1:A:177:TYR:CE2	2.01	0.95
1:A:253:MET:HE2	1:A:253:MET:HA	1.49	0.95
1:A:191:ASN:HB2	1:A:194:VAL:HG22	1.49	0.93
2:B:109:ARG:HG2	2:B:109:ARG:NH1	1.75	0.93
1:A:150:ASN:O	1:A:153:VAL:HG12	1.69	0.92
2:B:40:VAL:HG11	2:B:47:GLU:HG2	1.50	0.91
1:A:330:LYS:HD3	1:A:368:ILE:HG23	1.52	0.91
1:A:156:LEU:HD13	1:A:160:TYR:CD1	2.06	0.91
2:B:40:VAL:HG12	2:B:41:ILE:H	1.36	0.90
1:A:210:GLU:O	1:A:214:LYS:HB3	1.71	0.90
2:B:140:LEU:N	2:B:140:LEU:HD23	1.86	0.90
2:B:28:ASN:HB2	2:B:49:ARG:HG3	1.54	0.90
1:A:280:ARG:O	1:A:284:MET:HG3	1.72	0.88
2:B:217:LYS:HE2	2:B:217:LYS:H	1.34	0.88
2:B:95:VAL:HG13	2:B:99:GLY:HA3	1.56	0.88
2:B:118:VAL:HG21	2:B:126:PRO:HG3	1.55	0.86
1:A:294:GLY:HA3	1:A:313:VAL:HB	1.58	0.85
1:A:181:VAL:HG11	1:A:231:LEU:HD23	1.57	0.84
1:A:225:ILE:HG22	1:A:225:ILE:O	1.77	0.83
1:A:16:ILE:HG21	1:A:51:LEU:HD23	1.61	0.83
2:B:27:LYS:HZ1	2:B:29:LEU:HD13	1.42	0.83
2:B:109:ARG:HH11	2:B:109:ARG:CG	1.88	0.83
1:A:174:HIS:HB2	1:A:175:PRO:HD3	1.61	0.82
1:A:159:TRP:C	1:A:161:SER:H	1.85	0.82
2:B:156:GLN:HE22	2:B:178:VAL:HA	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG11	1:A:111:GLU:HG2	1.62	0.82
2:B:106:PHE:CD1	2:B:106:PHE:C	2.57	0.82
1:A:156:LEU:CD1	1:A:160:TYR:CD1	2.63	0.82
1:A:167:LEU:HD21	1:A:180:PHE:HD2	1.45	0.81
1:A:97:ARG:O	1:A:100:PRO:HD3	1.81	0.81
1:A:240:GLN:CD	1:A:244:LYS:HZ3	1.89	0.80
2:B:6:LYS:HZ1	2:B:11:GLY:N	1.78	0.80
1:A:8:PHE:HB2	1:A:67:VAL:HG12	1.64	0.79
2:B:3:GLU:HA	2:B:43:TRP:CZ3	2.18	0.79
2:B:28:ASN:HD22	2:B:49:ARG:HD3	1.48	0.79
2:B:53:PRO:HG2	2:B:215:TYR:HE1	1.48	0.77
1:A:220:MET:HE2	1:A:221:ASP:H	1.50	0.77
1:A:14:ARG:HG2	1:A:30:TYR:CE2	2.20	0.77
2:B:40:VAL:HG12	2:B:41:ILE:N	1.98	0.77
2:B:179:LYS:HD3	2:B:182:SER:HB2	1.65	0.77
2:B:51:TRP:HA	2:B:90:HIS:NE2	2.00	0.76
2:B:181:ARG:H	2:B:181:ARG:HD3	1.51	0.76
2:B:193:PHE:CE2	2:B:220:ALA:HB3	2.21	0.76
1:A:295:ALA:HB3	1:A:312:GLY:H	1.49	0.76
1:A:132:ASP:O	1:A:136:ILE:HG13	1.86	0.75
2:B:28:ASN:ND2	2:B:49:ARG:HD3	2.01	0.75
2:B:216:GLU:HB3	2:B:219:HIS:CD2	2.22	0.75
1:A:353:ILE:HD12	1:A:357:LEU:HD13	1.68	0.75
2:B:217:LYS:H	2:B:217:LYS:CE	2.00	0.74
2:B:106:PHE:C	2:B:106:PHE:HD1	1.95	0.74
1:A:240:GLN:NE2	1:A:240:GLN:HA	2.01	0.74
1:A:159:TRP:O	1:A:161:SER:N	2.22	0.73
2:B:6:LYS:HD2	2:B:7:HIS:H	1.54	0.72
2:B:181:ARG:HA	2:B:184:ASP:O	1.89	0.72
1:A:163:HIS:CD2	1:A:163:HIS:O	2.42	0.72
1:A:253:MET:HA	1:A:253:MET:CE	2.18	0.72
2:B:4:VAL:HG12	2:B:43:TRP:CE3	2.24	0.71
1:A:109:PHE:CD2	2:B:100:LYS:HD3	2.25	0.71
1:A:241:LEU:O	1:A:245:LEU:HG	1.90	0.71
1:A:214:LYS:HD2	1:A:215:THR:H	1.55	0.70
2:B:207:ILE:HB	2:B:223:VAL:O	1.91	0.70
1:A:167:LEU:HD23	1:A:177:TYR:HE2	1.54	0.70
1:A:240:GLN:CD	1:A:244:LYS:NZ	2.50	0.70
1:A:268:LEU:HD11	1:A:313:VAL:HG13	1.74	0.70
2:B:43:TRP:CD1	2:B:44:GLU:HG3	2.22	0.70
1:A:186:HIS:HD2	1:A:188:ASP:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:HIS:CE1	2:B:9:PHE:HD1	2.10	0.69
1:A:13:VAL:HG13	1:A:115:VAL:HG21	1.74	0.69
1:A:324:PRO:HB2	1:A:326:TRP:CD1	2.27	0.69
1:A:352:TYR:CE1	2:B:106:PHE:HZ	2.10	0.69
2:B:130:ASP:O	2:B:137:TYR:HE2	1.75	0.69
1:A:155:ARG:CB	1:A:155:ARG:HH21	2.05	0.68
1:A:214:LYS:HD2	1:A:215:THR:N	2.07	0.68
1:A:106:GLU:OE1	1:A:106:GLU:HA	1.92	0.68
2:B:51:TRP:CZ2	2:B:58:LEU:HB3	2.29	0.68
2:B:140:LEU:N	2:B:140:LEU:CD2	2.57	0.68
1:A:70:HIS:HB2	2:B:138:ARG:NH2	2.09	0.67
1:A:352:TYR:CG	2:B:106:PHE:CE1	2.82	0.67
1:A:180:PHE:CE1	1:A:184:VAL:HG21	2.29	0.67
1:A:76:ARG:HA	1:A:79:GLU:HG2	1.76	0.66
2:B:53:PRO:CG	2:B:215:TYR:HE1	2.07	0.66
1:A:67:VAL:HG23	1:A:85:THR:HG23	1.76	0.66
2:B:28:ASN:HB2	2:B:49:ARG:CG	2.25	0.66
2:B:40:VAL:CG1	2:B:47:GLU:HG2	2.23	0.66
1:A:167:LEU:CD2	1:A:180:PHE:HD2	2.08	0.66
2:B:147:ILE:HG13	2:B:168:LEU:HD13	1.77	0.66
1:A:88:PHE:CD1	1:A:89:PRO:HA	2.31	0.66
2:B:81:GLY:O	2:B:83:ALA:N	2.29	0.66
2:B:140:LEU:HD23	2:B:140:LEU:H	1.60	0.65
2:B:13:TYR:HE2	2:B:27:LYS:HB3	1.62	0.65
2:B:88:ALA:HA	2:B:91:VAL:HG13	1.78	0.65
1:A:150:ASN:ND2	1:A:151:LEU:HD13	2.11	0.65
2:B:38:GLU:CD	2:B:49:ARG:HH21	2.05	0.65
1:A:294:GLY:HA3	1:A:313:VAL:H	1.62	0.65
2:B:179:LYS:HE2	2:B:181:ARG:HG2	1.78	0.65
2:B:3:GLU:HA	2:B:43:TRP:CH2	2.32	0.64
1:A:119:LEU:HD11	1:A:123:ARG:NE	2.12	0.64
1:A:159:TRP:C	1:A:161:SER:N	2.51	0.64
1:A:163:HIS:O	1:A:163:HIS:HD2	1.80	0.63
1:A:240:GLN:O	1:A:244:LYS:HD3	1.98	0.63
2:B:161:ILE:O	2:B:165:LYS:HG3	1.98	0.63
1:A:14:ARG:CG	1:A:30:TYR:CE2	2.81	0.63
1:A:181:VAL:HG11	1:A:231:LEU:CD2	2.26	0.63
1:A:174:HIS:CD2	1:A:174:HIS:H	2.15	0.63
2:B:2:VAL:O	2:B:43:TRP:HZ3	1.81	0.63
2:B:40:VAL:CG1	2:B:41:ILE:H	2.11	0.63
1:A:160:TYR:HD2	1:A:161:SER:N	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LYS:HE3	1:A:266:ALA:HB2	1.81	0.63
1:A:13:VAL:HG21	1:A:112:TYR:HA	1.81	0.63
1:A:167:LEU:HB3	1:A:177:TYR:OH	1.98	0.62
1:A:8:PHE:HD1	1:A:19:PHE:O	1.82	0.62
1:A:136:ILE:O	1:A:140:GLU:HG2	1.98	0.62
1:A:294:GLY:CA	1:A:313:VAL:HB	2.28	0.62
1:A:220:MET:CE	1:A:221:ASP:H	2.11	0.62
1:A:352:TYR:CD1	2:B:106:PHE:CE1	2.87	0.62
2:B:7:HIS:CE1	2:B:9:PHE:CD1	2.87	0.62
1:A:225:ILE:O	1:A:225:ILE:CG2	2.48	0.62
2:B:80:LEU:HD12	2:B:149:GLU:HB2	1.82	0.62
2:B:151:VAL:CG2	2:B:153:GLN:HG2	2.30	0.62
1:A:157:ARG:O	1:A:160:TYR:CE2	2.53	0.62
1:A:69:GLU:CD	1:A:97:ARG:HH12	2.08	0.61
2:B:221:LEU:HD12	2:B:221:LEU:O	2.00	0.61
1:A:257:ALA:HB1	1:A:260:LEU:HB2	1.82	0.61
2:B:29:LEU:HG	2:B:97:TRP:CZ2	2.35	0.61
1:A:220:MET:HB3	1:A:223:THR:HB	1.82	0.61
1:A:47:ILE:HG23	1:A:51:LEU:HD12	1.82	0.61
2:B:104:ILE:HG22	2:B:104:ILE:O	2.01	0.61
1:A:8:PHE:O	1:A:92:ALA:HB2	2.01	0.61
1:A:240:GLN:NE2	1:A:244:LYS:HD3	2.15	0.61
1:A:143:ASP:O	1:A:151:LEU:HD22	2.00	0.61
2:B:42:LYS:HD3	2:B:42:LYS:N	2.15	0.61
1:A:280:ARG:NH2	1:A:284:MET:HE1	2.16	0.60
1:A:109:PHE:HD2	2:B:100:LYS:HD3	1.67	0.60
2:B:27:LYS:O	2:B:27:LYS:HG3	2.01	0.60
2:B:193:PHE:HE2	2:B:220:ALA:HB3	1.67	0.60
1:A:36:GLU:HG2	1:A:118:ALA:HB3	1.83	0.60
1:A:225:ILE:HA	1:A:228:VAL:HG22	1.83	0.60
2:B:6:LYS:HZ1	2:B:11:GLY:H	1.49	0.60
2:B:179:LYS:HB3	2:B:182:SER:CB	2.32	0.60
1:A:317:TYR:CD1	1:A:318:PRO:HD2	2.37	0.60
2:B:52:ASN:OD1	2:B:52:ASN:C	2.44	0.60
1:A:156:LEU:CD1	1:A:160:TYR:HD1	2.13	0.60
2:B:86:THR:C	2:B:88:ALA:H	2.08	0.60
1:A:352:TYR:CD1	2:B:106:PHE:CZ	2.90	0.59
1:A:13:VAL:CG1	1:A:13:VAL:O	2.50	0.59
1:A:36:GLU:HG2	1:A:118:ALA:CB	2.31	0.59
1:A:186:HIS:CE1	1:A:219:TRP:HE3	2.20	0.59
1:A:197:GLU:O	1:A:198:LEU:CB	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:CD1	1:A:357:LEU:HD13	2.32	0.59
2:B:36:TYR:O	2:B:36:TYR:CD2	2.55	0.59
2:B:100:LYS:C	2:B:101:ILE:HD12	2.27	0.59
1:A:156:LEU:HD22	1:A:156:LEU:O	2.01	0.59
1:A:93:GLY:HA3	1:A:97:ARG:NH1	2.18	0.58
2:B:61:ALA:HB2	2:B:221:LEU:HD23	1.84	0.58
1:A:8:PHE:CD1	1:A:19:PHE:O	2.56	0.58
1:A:167:LEU:HD21	1:A:180:PHE:CD2	2.33	0.58
2:B:3:GLU:HA	2:B:43:TRP:HZ3	1.66	0.58
1:A:365:ILE:HA	1:A:368:ILE:HG12	1.85	0.58
2:B:53:PRO:CG	2:B:215:TYR:CE1	2.86	0.58
2:B:216:GLU:CB	2:B:219:HIS:CD2	2.87	0.58
1:A:155:ARG:HH21	1:A:155:ARG:CA	2.17	0.58
1:A:356:GLU:O	1:A:360:GLU:HG3	2.04	0.58
2:B:53:PRO:HG2	2:B:215:TYR:CE1	2.35	0.58
1:A:225:ILE:HA	1:A:228:VAL:CG2	2.34	0.58
2:B:123:ASN:CG	2:B:123:ASN:O	2.47	0.58
1:A:180:PHE:CZ	1:A:190:ILE:HD11	2.39	0.58
2:B:38:GLU:OE1	2:B:49:ARG:HD2	2.04	0.58
2:B:40:VAL:HG11	2:B:47:GLU:CG	2.30	0.57
2:B:39:ARG:O	2:B:50:ILE:HB	2.04	0.57
2:B:35:VAL:O	2:B:36:TYR:CD1	2.57	0.57
2:B:175:MET:HE2	2:B:221:LEU:HD11	1.85	0.57
1:A:275:LEU:HD11	1:A:313:VAL:HG21	1.86	0.57
1:A:235:ILE:HG22	1:A:240:GLN:N	2.19	0.57
1:A:164:PHE:CD1	1:A:167:LEU:HB2	2.40	0.57
1:A:315:TYR:HD1	1:A:320:ILE:HG21	1.70	0.57
1:A:172:PRO:HD2	1:A:176:GLN:OE1	2.05	0.57
2:B:6:LYS:NZ	2:B:11:GLY:N	2.52	0.57
2:B:61:ALA:CB	2:B:221:LEU:HD23	2.35	0.57
1:A:275:LEU:HD22	1:A:293:LEU:HD22	1.87	0.56
1:A:221:ASP:OD2	1:A:221:ASP:O	2.24	0.56
1:A:74:SER:OG	1:A:86:THR:HB	2.05	0.56
2:B:24:ILE:HG22	2:B:25:ALA:N	2.21	0.56
1:A:195:LEU:O	1:A:200:LEU:HB2	2.05	0.56
1:A:160:TYR:C	1:A:160:TYR:CD2	2.84	0.56
1:A:96:LEU:HD13	1:A:103:PHE:CE1	2.40	0.56
1:A:195:LEU:HD13	1:A:200:LEU:HD23	1.87	0.56
2:B:27:LYS:O	2:B:93:ASP:HB3	2.06	0.56
1:A:12:ASN:O	1:A:31:PHE:HE2	1.89	0.56
1:A:191:ASN:HB2	1:A:194:VAL:CG2	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ILE:O	1:A:369:LYS:HD3	2.06	0.56
2:B:210:LEU:HD12	2:B:211:ASN:N	2.21	0.56
2:B:9:PHE:HZ	2:B:66:LEU:O	1.89	0.56
1:A:17:TYR:CE2	1:A:28:LYS:HD3	2.40	0.55
1:A:160:TYR:HD2	1:A:160:TYR:C	2.14	0.55
1:A:13:VAL:O	1:A:13:VAL:HG12	2.06	0.55
1:A:142:LEU:HD11	1:A:246:GLU:HG3	1.89	0.55
1:A:187:ARG:O	1:A:190:ILE:HG12	2.06	0.55
2:B:147:ILE:CD1	2:B:164:ALA:HA	2.36	0.55
2:B:215:TYR:C	2:B:216:GLU:HG2	2.30	0.55
1:A:174:HIS:CD2	1:A:174:HIS:N	2.74	0.55
2:B:27:LYS:NZ	2:B:29:LEU:HD13	2.17	0.55
2:B:79:TYR:C	2:B:79:TYR:HD2	2.15	0.55
1:A:131:ARG:HG3	1:A:134:MET:HE2	1.88	0.55
2:B:95:VAL:HG13	2:B:99:GLY:CA	2.34	0.55
2:B:148:PHE:HD1	2:B:175:MET:HB2	1.72	0.55
2:B:6:LYS:NZ	2:B:11:GLY:H	2.04	0.55
2:B:127:ILE:HG12	2:B:140:LEU:HD12	1.89	0.55
1:A:352:TYR:CE1	2:B:106:PHE:CZ	2.93	0.54
1:A:191:ASN:O	1:A:195:LEU:HB2	2.07	0.54
1:A:251:ARG:HG3	1:A:251:ARG:HH11	1.71	0.54
1:A:352:TYR:CZ	1:A:354:ALA:HB3	2.42	0.54
1:A:72:GLU:OE1	1:A:72:GLU:HA	2.08	0.54
2:B:106:PHE:HB2	2:B:129:GLY:O	2.08	0.54
1:A:170:LEU:O	1:A:172:PRO:HD3	2.08	0.54
1:A:72:GLU:HG3	1:A:76:ARG:HD2	1.88	0.54
1:A:96:LEU:HD13	1:A:103:PHE:CD1	2.42	0.54
1:A:38:VAL:HG12	1:A:48:THR:HG21	1.88	0.54
2:B:151:VAL:HG23	2:B:153:GLN:HG2	1.89	0.54
2:B:115:VAL:O	2:B:118:VAL:HG23	2.08	0.53
2:B:36:TYR:O	2:B:36:TYR:HD2	1.91	0.53
1:A:49:LYS:O	1:A:53:GLU:HG3	2.08	0.53
1:A:226:GLU:OE1	1:A:226:GLU:HA	2.09	0.53
1:A:311:HIS:CE1	1:A:325:TRP:CH2	2.96	0.53
1:A:177:TYR:C	1:A:179:ALA:H	2.14	0.53
2:B:181:ARG:HD3	2:B:181:ARG:N	2.21	0.53
2:B:206:VAL:HG12	2:B:206:VAL:O	2.09	0.53
1:A:20:ASP:OD2	1:A:24:ASN:N	2.39	0.53
1:A:109:PHE:O	1:A:112:TYR:N	2.41	0.53
1:A:240:GLN:HA	1:A:240:GLN:HE21	1.70	0.53
1:A:240:GLN:HG3	1:A:244:LYS:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLN:HE21	1:A:244:LYS:HD3	1.73	0.53
2:B:79:TYR:C	2:B:79:TYR:CD2	2.86	0.53
2:B:179:LYS:HB3	2:B:182:SER:HB2	1.89	0.53
1:A:155:ARG:HA	1:A:155:ARG:NH2	2.24	0.53
1:A:214:LYS:CD	1:A:215:THR:N	2.72	0.53
2:B:28:ASN:HB3	2:B:47:GLU:O	2.09	0.53
1:A:251:ARG:HG3	1:A:251:ARG:NH1	2.24	0.52
2:B:181:ARG:H	2:B:181:ARG:CD	2.13	0.52
1:A:142:LEU:HD12	1:A:245:LEU:HB2	1.91	0.52
2:B:31:PRO:HA	2:B:47:GLU:OE1	2.08	0.52
1:A:96:LEU:HA	1:A:103:PHE:CE1	2.44	0.52
1:A:109:PHE:O	1:A:110:GLU:C	2.52	0.52
2:B:82:ILE:O	2:B:83:ALA:O	2.28	0.52
1:A:130:ALA:HB1	1:A:133:LYS:HG2	1.90	0.52
1:A:180:PHE:CE1	1:A:190:ILE:HD11	2.45	0.52
2:B:4:VAL:HG12	2:B:43:TRP:CD2	2.44	0.52
1:A:34:LYS:O	1:A:38:VAL:HG23	2.10	0.52
2:B:62:ILE:HG22	2:B:63:VAL:N	2.25	0.52
1:A:356:GLU:OE2	2:B:152:ALA:HB1	2.09	0.52
1:A:47:ILE:HG12	1:A:73:LEU:HD12	1.92	0.52
1:A:113:TYR:CD2	1:A:114:LYS:N	2.78	0.52
1:A:359:LYS:HE2	2:B:184:ASP:HA	1.92	0.52
2:B:27:LYS:HZ1	2:B:29:LEU:CD1	2.17	0.52
1:A:161:SER:C	1:A:164:PHE:H	2.18	0.52
1:A:141:ALA:HB3	1:A:245:LEU:HD13	1.91	0.51
2:B:25:ALA:HA	2:B:49:ARG:O	2.10	0.51
1:A:153:VAL:CG1	1:A:154:ALA:N	2.73	0.51
2:B:2:VAL:O	2:B:43:TRP:CZ3	2.62	0.51
2:B:74:GLY:O	2:B:99:GLY:HA2	2.10	0.51
2:B:123:ASN:C	2:B:124:ILE:HG13	2.35	0.51
2:B:130:ASP:OD1	2:B:132:THR:HG23	2.09	0.51
2:B:121:ARG:C	2:B:123:ASN:H	2.18	0.51
2:B:193:PHE:CE2	2:B:220:ALA:CB	2.93	0.51
1:A:161:SER:O	1:A:164:PHE:N	2.42	0.51
1:A:266:ALA:O	1:A:269:ALA:HB3	2.11	0.51
1:A:295:ALA:HB3	1:A:312:GLY:N	2.22	0.51
2:B:17:ASP:OD1	2:B:17:ASP:N	2.44	0.51
2:B:113:GLU:O	2:B:116:PRO:HD2	2.10	0.51
2:B:161:ILE:O	2:B:164:ALA:HB3	2.11	0.51
2:B:217:LYS:HE2	2:B:217:LYS:N	2.13	0.51
1:A:231:LEU:N	1:A:231:LEU:HD22	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:HG3	1:A:30:TYR:CD2	2.45	0.51
2:B:147:ILE:HD12	2:B:164:ALA:HA	1.91	0.51
1:A:32:THR:HG23	1:A:50:ASP:OD2	2.10	0.51
1:A:182:LYS:HG2	1:A:231:LEU:HB3	1.93	0.50
2:B:51:TRP:CG	2:B:90:HIS:CD2	2.99	0.50
2:B:28:ASN:HB2	2:B:49:ARG:CD	2.41	0.50
2:B:141:VAL:HG23	2:B:142:THR:N	2.26	0.50
1:A:43:LEU:HD21	2:B:139:ALA:HB3	1.92	0.50
1:A:170:LEU:N	1:A:170:LEU:HD12	2.26	0.50
1:A:171:LEU:HD23	1:A:171:LEU:N	2.26	0.50
2:B:7:HIS:HE1	2:B:9:PHE:CD1	2.30	0.50
2:B:110:VAL:HG12	2:B:111:LEU:N	2.26	0.50
1:A:171:LEU:O	1:A:177:TYR:CD1	2.64	0.50
2:B:115:VAL:HB	2:B:116:PRO:HD3	1.92	0.50
2:B:77:VAL:HG22	2:B:101:ILE:HG13	1.93	0.50
1:A:180:PHE:O	1:A:184:VAL:HG22	2.12	0.50
2:B:42:LYS:HA	2:B:46:GLU:O	2.12	0.50
1:A:171:LEU:HD12	1:A:177:TYR:HA	1.94	0.50
1:A:202:GLU:O	1:A:205:ILE:HG22	2.12	0.50
2:B:24:ILE:HG13	2:B:63:VAL:HG23	1.94	0.50
2:B:173:TYR:CE1	2:B:225:ARG:HD2	2.47	0.50
1:A:78:LYS:C	1:A:80:LEU:H	2.17	0.50
2:B:198:ARG:HE	2:B:199:GLU:N	2.10	0.50
2:B:106:PHE:CD1	2:B:106:PHE:O	2.65	0.49
2:B:155:THR:O	2:B:156:GLN:C	2.55	0.49
1:A:163:HIS:CE1	1:A:187:ARG:H	2.30	0.49
2:B:79:TYR:CD1	2:B:82:ILE:HD12	2.47	0.49
2:B:131:ALA:HA	2:B:137:TYR:OH	2.12	0.49
1:A:34:LYS:HB3	1:A:36:GLU:OE1	2.13	0.49
1:A:108:TRP:CZ2	2:B:100:LYS:HE3	2.47	0.49
1:A:210:GLU:CD	1:A:214:LYS:HG2	2.37	0.49
2:B:185:VAL:HG22	2:B:185:VAL:O	2.11	0.49
1:A:291:GLN:HA	1:A:314:ILE:HD11	1.94	0.49
2:B:5:LYS:NZ	2:B:16:ILE:HD12	2.27	0.49
1:A:263:LEU:HD12	1:A:342:ALA:HB2	1.93	0.49
1:A:271:ARG:O	1:A:275:LEU:HB2	2.13	0.49
2:B:218:ASP:N	2:B:218:ASP:OD2	2.43	0.49
2:B:104:ILE:O	2:B:104:ILE:CG2	2.61	0.49
2:B:207:ILE:HG22	2:B:208:GLU:HB3	1.93	0.49
1:A:177:TYR:C	1:A:179:ALA:N	2.68	0.49
1:A:342:ALA:O	1:A:346:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LEU:O	2:B:59:GLY:C	2.55	0.49
1:A:11:GLU:OE2	1:A:11:GLU:N	2.45	0.49
2:B:35:VAL:O	2:B:38:GLU:HG2	2.12	0.49
2:B:62:ILE:CG2	2:B:63:VAL:N	2.76	0.49
2:B:78:LEU:HB2	2:B:144:VAL:HG11	1.94	0.49
2:B:118:VAL:HG21	2:B:126:PRO:CG	2.34	0.49
2:B:221:LEU:HD12	2:B:221:LEU:C	2.38	0.49
2:B:6:LYS:HD3	2:B:13:TYR:CE1	2.48	0.49
2:B:40:VAL:O	2:B:41:ILE:HG23	2.12	0.48
1:A:188:ASP:HA	1:A:212:LYS:HG3	1.96	0.48
1:A:203:GLU:O	1:A:207:LYS:HD3	2.14	0.48
2:B:2:VAL:O	2:B:2:VAL:HG23	2.13	0.48
2:B:10:PRO:HB2	2:B:73:PRO:HD3	1.96	0.48
2:B:151:VAL:HG23	2:B:153:GLN:H	1.77	0.48
1:A:8:PHE:HD2	1:A:66:PHE:HA	1.78	0.48
1:A:113:TYR:CD2	1:A:113:TYR:C	2.91	0.48
2:B:95:VAL:HG12	2:B:96:GLY:N	2.29	0.48
2:B:106:PHE:CB	2:B:129:GLY:O	2.62	0.48
1:A:113:TYR:HD2	1:A:114:LYS:N	2.11	0.48
1:A:208:ILE:O	1:A:211:ALA:HB3	2.14	0.48
2:B:51:TRP:HE1	2:B:56:SER:CB	2.26	0.48
1:A:285:MET:SD	1:A:289:THR:HG22	2.53	0.48
1:A:108:TRP:CH2	2:B:100:LYS:HE3	2.48	0.48
2:B:56:SER:HB2	2:B:87:THR:HA	1.95	0.48
1:A:113:TYR:O	1:A:114:LYS:C	2.57	0.48
2:B:36:TYR:OH	2:B:50:ILE:O	2.31	0.48
2:B:38:GLU:CD	2:B:49:ARG:HD2	2.39	0.48
2:B:135:GLU:O	2:B:138:ARG:HG2	2.14	0.48
2:B:28:ASN:HB2	2:B:49:ARG:HD3	1.96	0.47
2:B:6:LYS:HD2	2:B:12:VAL:O	2.14	0.47
1:A:149:ILE:HG22	1:A:242:ARG:HH11	1.79	0.47
2:B:38:GLU:CD	2:B:49:ARG:NH2	2.71	0.47
2:B:38:GLU:OE2	2:B:49:ARG:NH2	2.47	0.47
1:A:156:LEU:HD11	1:A:160:TYR:HD1	1.79	0.47
2:B:100:LYS:O	2:B:101:ILE:HD12	2.13	0.47
2:B:156:GLN:HG3	2:B:183:ILE:HD11	1.96	0.47
1:A:243:LYS:O	1:A:244:LYS:C	2.56	0.47
1:A:355:GLU:HB3	2:B:154:PRO:HD3	1.96	0.47
2:B:162:ASP:HA	2:B:165:LYS:HG3	1.95	0.47
1:A:67:VAL:HG13	1:A:67:VAL:O	2.15	0.47
1:A:78:LYS:HA	1:A:82:PHE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:VAL:HG13	1:A:231:LEU:HD12	1.97	0.47
2:B:125:ILE:HG22	2:B:127:ILE:HG13	1.96	0.47
1:A:167:LEU:CD2	1:A:180:PHE:CD2	2.94	0.46
1:A:156:LEU:HD11	1:A:160:TYR:CD1	2.50	0.46
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.80	0.46
1:A:112:TYR:O	2:B:125:ILE:HD13	2.15	0.46
1:A:184:VAL:CG2	1:A:185:GLY:N	2.77	0.46
1:A:240:GLN:NE2	1:A:240:GLN:CA	2.77	0.46
2:B:145:ASP:OD2	2:B:169:LYS:NZ	2.33	0.46
1:A:150:ASN:CG	1:A:151:LEU:HD13	2.41	0.46
1:A:164:PHE:CE1	1:A:167:LEU:HD13	2.50	0.46
1:A:186:HIS:CD2	1:A:188:ASP:H	2.26	0.46
1:A:18:ALA:O	1:A:25:LEU:HD23	2.16	0.46
1:A:197:GLU:O	1:A:198:LEU:HB3	2.13	0.46
2:B:51:TRP:CD1	2:B:90:HIS:CD2	3.04	0.46
1:A:40:ASP:HB2	1:A:122:MET:HE1	1.98	0.46
1:A:168:ASP:HA	1:A:177:TYR:HE1	1.79	0.46
1:A:215:THR:HG23	1:A:216:MET:N	2.29	0.46
1:A:117:VAL:O	1:A:118:ALA:C	2.58	0.46
1:A:173:LYS:HB3	1:A:176:GLN:HG2	1.96	0.46
2:B:168:LEU:HD23	2:B:226:LYS:HD2	1.97	0.46
2:B:170:ARG:NH1	2:B:170:ARG:HB3	2.31	0.46
1:A:131:ARG:HD3	1:A:252:ALA:HB1	1.98	0.46
2:B:77:VAL:HB	2:B:146:VAL:O	2.15	0.46
2:B:151:VAL:CG2	2:B:153:GLN:CG	2.93	0.46
1:A:155:ARG:HH21	1:A:155:ARG:CG	2.29	0.46
1:A:163:HIS:NE2	1:A:187:ARG:HB3	2.30	0.46
1:A:195:LEU:HD12	1:A:205:ILE:HA	1.98	0.46
1:A:210:GLU:HG2	1:A:214:LYS:HB3	1.98	0.46
2:B:78:LEU:N	2:B:144:VAL:HG11	2.31	0.46
2:B:209:ARG:HG3	2:B:222:PHE:CZ	2.50	0.46
1:A:139:ILE:HG22	1:A:140:GLU:N	2.31	0.46
1:A:220:MET:HG3	1:A:223:THR:OG1	2.16	0.45
1:A:224:ASP:O	1:A:228:VAL:HG22	2.16	0.45
1:A:285:MET:HA	1:A:286:PRO:HD2	1.73	0.45
2:B:53:PRO:O	2:B:56:SER:O	2.34	0.45
2:B:79:TYR:CE1	2:B:88:ALA:HB2	2.51	0.45
1:A:153:VAL:HG23	1:A:234:GLU:OE2	2.16	0.45
1:A:251:ARG:HG3	1:A:251:ARG:O	2.15	0.45
1:A:251:ARG:O	1:A:251:ARG:CG	2.64	0.45
2:B:88:ALA:HA	2:B:91:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:GLN:CB	2:B:176:ILE:HD11	2.46	0.45
1:A:8:PHE:CZ	1:A:65:GLU:CD	2.95	0.45
1:A:12:ASN:OD1	1:A:17:TYR:HE1	1.98	0.45
2:B:82:ILE:O	2:B:83:ALA:C	2.59	0.45
1:A:186:HIS:CE1	1:A:219:TRP:CE3	3.02	0.45
1:A:221:ASP:OD2	1:A:221:ASP:C	2.60	0.45
1:A:70:HIS:HB2	2:B:138:ARG:HH22	1.79	0.45
1:A:141:ALA:O	1:A:144:ASP:N	2.48	0.45
1:A:164:PHE:HD1	1:A:167:LEU:HB2	1.81	0.45
2:B:160:LEU:HD12	2:B:160:LEU:O	2.17	0.45
1:A:178:VAL:HG12	1:A:182:LYS:HG3	1.99	0.45
1:A:192:GLU:HG3	1:A:205:ILE:CD1	2.46	0.45
2:B:86:THR:C	2:B:88:ALA:N	2.75	0.45
1:A:33:ASP:O	1:A:34:LYS:C	2.60	0.45
2:B:179:LYS:HB3	2:B:182:SER:HB3	1.98	0.45
1:A:279:LEU:O	1:A:280:ARG:C	2.60	0.44
2:B:36:TYR:CD2	2:B:36:TYR:C	2.95	0.44
1:A:231:LEU:HD13	1:A:231:LEU:HA	1.61	0.44
1:A:280:ARG:HG3	1:A:347:TYR:CZ	2.52	0.44
2:B:156:GLN:HB3	2:B:176:ILE:HD11	1.99	0.44
1:A:42:LEU:HD21	1:A:51:LEU:HB2	1.99	0.44
1:A:161:SER:HA	1:A:164:PHE:O	2.17	0.44
1:A:164:PHE:HE1	1:A:167:LEU:HD13	1.83	0.44
1:A:156:LEU:HD22	1:A:159:TRP:HB3	1.98	0.44
1:A:178:VAL:HG12	1:A:178:VAL:O	2.17	0.44
2:B:214:PRO:HD2	2:B:215:TYR:HD2	1.82	0.44
1:A:220:MET:SD	1:A:222:GLN:N	2.86	0.44
1:A:364:ARG:O	1:A:368:ILE:HG12	2.17	0.44
2:B:73:PRO:HA	2:B:95:VAL:HA	1.98	0.44
2:B:110:VAL:O	2:B:111:LEU:C	2.61	0.44
2:B:151:VAL:C	2:B:153:GLN:H	2.26	0.44
2:B:161:ILE:O	2:B:165:LYS:CG	2.63	0.44
1:A:167:LEU:O	1:A:168:ASP:C	2.61	0.44
1:A:16:ILE:HD12	1:A:51:LEU:HA	1.99	0.44
1:A:42:LEU:HG	1:A:48:THR:CG2	2.48	0.44
1:A:141:ALA:HB3	1:A:245:LEU:CD1	2.48	0.43
1:A:153:VAL:HG13	1:A:154:ALA:N	2.33	0.43
1:A:101:GLU:HB3	1:A:108:TRP:CD1	2.53	0.43
1:A:164:PHE:CZ	1:A:166:GLU:HB2	2.53	0.43
1:A:29:ARG:HH22	1:A:53:GLU:CB	2.30	0.43
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TYR:CD1	1:A:320:ILE:HG21	2.53	0.43
1:A:96:LEU:HD13	1:A:96:LEU:HA	1.68	0.43
1:A:240:GLN:NE2	1:A:244:LYS:CD	2.81	0.43
1:A:90:ASN:O	1:A:90:ASN:OD1	2.36	0.43
1:A:15:GLY:HA2	1:A:31:PHE:CE2	2.53	0.43
2:B:53:PRO:HB2	2:B:215:TYR:CD1	2.53	0.43
1:A:109:PHE:CD1	1:A:109:PHE:C	2.96	0.43
1:A:334:ALA:O	1:A:338:LYS:HG2	2.18	0.43
2:B:139:ALA:C	2:B:140:LEU:HD23	2.42	0.43
2:B:217:LYS:O	2:B:219:HIS:CD2	2.72	0.43
1:A:161:SER:C	1:A:163:HIS:N	2.77	0.43
1:A:325:TRP:CE3	1:A:328:ARG:HD2	2.54	0.43
2:B:73:PRO:HG3	2:B:94:ILE:O	2.18	0.43
2:B:97:TRP:CZ3	2:B:123:ASN:HB2	2.53	0.43
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.73	0.43
1:A:163:HIS:CD2	1:A:163:HIS:C	2.96	0.43
1:A:195:LEU:HB3	1:A:205:ILE:CD1	2.48	0.43
1:A:235:ILE:HD13	1:A:235:ILE:HA	1.74	0.43
1:A:352:TYR:CD1	2:B:106:PHE:HE1	2.34	0.43
1:A:132:ASP:OD2	1:A:132:ASP:N	2.51	0.42
1:A:38:VAL:CG1	1:A:48:THR:HG21	2.50	0.42
2:B:51:TRP:HZ2	2:B:58:LEU:HB3	1.81	0.42
1:A:8:PHE:O	1:A:92:ALA:CB	2.67	0.42
1:A:187:ARG:HG3	1:A:188:ASP:OD2	2.19	0.42
1:A:347:TYR:CD1	1:A:347:TYR:C	2.95	0.42
2:B:204:PHE:CD1	2:B:224:VAL:HG11	2.54	0.42
1:A:353:ILE:CD1	1:A:357:LEU:CD1	2.96	0.42
2:B:39:ARG:HG3	2:B:50:ILE:HG12	2.01	0.42
2:B:214:PRO:HD2	2:B:215:TYR:CD2	2.55	0.42
1:A:78:LYS:C	1:A:80:LEU:N	2.78	0.42
2:B:22:GLU:C	2:B:23:LYS:HG2	2.45	0.42
2:B:194:LYS:O	2:B:198:ARG:HB2	2.19	0.42
1:A:181:VAL:CG1	1:A:231:LEU:HD23	2.40	0.42
1:A:353:ILE:HD12	1:A:353:ILE:O	2.19	0.42
2:B:130:ASP:O	2:B:137:TYR:CE2	2.65	0.42
2:B:180:SER:HB3	2:B:218:ASP:HB2	2.01	0.42
1:A:178:VAL:HG13	1:A:231:LEU:HB3	2.02	0.42
1:A:323:SER:HB3	1:A:324:PRO:HD2	2.02	0.42
2:B:173:TYR:CZ	2:B:225:ARG:HD2	2.55	0.42
1:A:119:LEU:HD11	1:A:123:ARG:CD	2.49	0.42
1:A:150:ASN:OD1	1:A:150:ASN:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:O	1:A:243:LYS:C	2.63	0.42
2:B:40:VAL:CG1	2:B:41:ILE:N	2.68	0.42
2:B:196:VAL:O	2:B:200:LEU:HB2	2.20	0.42
1:A:90:ASN:OD1	1:A:90:ASN:C	2.63	0.42
1:A:130:ALA:HB1	1:A:133:LYS:CG	2.50	0.42
1:A:151:LEU:HD13	1:A:151:LEU:N	2.34	0.42
1:A:155:ARG:HH21	1:A:155:ARG:HA	1.81	0.42
1:A:166:GLU:O	1:A:167:LEU:C	2.62	0.42
2:B:27:LYS:O	2:B:27:LYS:CG	2.67	0.42
2:B:176:ILE:HG12	2:B:178:VAL:CG2	2.50	0.42
1:A:9:ILE:HD11	1:A:58:LEU:HD11	2.01	0.42
2:B:176:ILE:HG12	2:B:178:VAL:HG23	2.02	0.42
1:A:170:LEU:N	1:A:170:LEU:CD1	2.83	0.41
1:A:186:HIS:NE2	1:A:219:TRP:HE3	2.18	0.41
1:A:214:LYS:O	1:A:215:THR:HB	2.20	0.41
1:A:268:LEU:CD1	1:A:313:VAL:HG13	2.47	0.41
1:A:368:ILE:O	1:A:368:ILE:HG22	2.20	0.41
2:B:220:ALA:O	2:B:222:PHE:HD1	2.04	0.41
1:A:14:ARG:HG3	1:A:30:TYR:CE2	2.56	0.41
1:A:240:GLN:HE21	1:A:240:GLN:CA	2.34	0.41
2:B:27:LYS:HZ1	2:B:29:LEU:HB2	1.84	0.41
2:B:27:LYS:NZ	2:B:29:LEU:HB2	2.35	0.41
1:A:177:TYR:C	1:A:177:TYR:CD2	2.99	0.41
2:B:35:VAL:O	2:B:38:GLU:CG	2.68	0.41
2:B:76:SER:CB	2:B:100:LYS:HB2	2.49	0.41
1:A:164:PHE:CE1	1:A:167:LEU:HB2	2.55	0.41
1:A:184:VAL:HG23	1:A:185:GLY:N	2.34	0.41
1:A:36:GLU:HG2	1:A:118:ALA:HB1	2.02	0.41
1:A:51:LEU:HD13	1:A:51:LEU:O	2.21	0.41
1:A:181:VAL:O	1:A:182:LYS:C	2.64	0.41
1:A:182:LYS:HG2	1:A:231:LEU:CB	2.50	0.41
1:A:313:VAL:O	1:A:316:GLN:HG3	2.21	0.41
1:A:330:LYS:HE2	1:A:368:ILE:HD12	2.01	0.41
2:B:38:GLU:OE2	2:B:49:ARG:HD2	2.20	0.41
2:B:116:PRO:O	2:B:117:ILE:C	2.62	0.41
2:B:156:GLN:HG3	2:B:183:ILE:CD1	2.51	0.41
2:B:184:ASP:CG	2:B:187:LYS:HB2	2.46	0.41
1:A:20:ASP:O	1:A:22:ASN:N	2.54	0.41
1:A:155:ARG:HH21	1:A:155:ARG:HB3	1.85	0.41
1:A:271:ARG:CG	1:A:275:LEU:HD12	2.51	0.41
2:B:71:ILE:HD11	2:B:175:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:THR:O	2:B:143:LYS:C	2.64	0.41
1:A:149:ILE:O	1:A:150:ASN:C	2.63	0.40
1:A:156:LEU:HD13	1:A:160:TYR:CE1	2.54	0.40
1:A:177:TYR:C	1:A:177:TYR:HD2	2.29	0.40
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.84	0.40
1:A:352:TYR:CG	2:B:106:PHE:CZ	3.09	0.40
2:B:17:ASP:HB2	2:B:18:ASP:H	1.70	0.40
1:A:131:ARG:HA	1:A:134:MET:SD	2.62	0.40
1:A:160:TYR:CZ	1:A:177:TYR:CZ	3.10	0.40
1:A:195:LEU:HD21	1:A:208:ILE:CG2	2.51	0.40
2:B:7:HIS:ND1	2:B:9:PHE:HD1	2.18	0.40
1:A:14:ARG:HG2	1:A:30:TYR:CZ	2.57	0.40
1:A:69:GLU:OE2	1:A:97:ARG:NH1	2.54	0.40
1:A:190:ILE:HG23	1:A:195:LEU:HD23	2.04	0.40
2:B:111:LEU:O	2:B:113:GLU:N	2.54	0.40
2:B:160:LEU:HD12	2:B:160:LEU:C	2.46	0.40
1:A:137:GLN:O	1:A:140:GLU:N	2.55	0.40
1:A:155:ARG:NH2	1:A:155:ARG:CG	2.84	0.40
2:B:35:VAL:O	2:B:36:TYR:CG	2.75	0.40
2:B:176:ILE:O	2:B:176:ILE:HG23	2.22	0.40
1:A:160:TYR:CD2	1:A:161:SER:N	2.84	0.40
1:A:170:LEU:C	1:A:171:LEU:HD23	2.46	0.40
1:A:335:LEU:HD22	1:A:339:LEU:HD11	2.04	0.40
2:B:16:ILE:HD13	2:B:16:ILE:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	338/371 (91%)	281 (83%)	44 (13%)	13 (4%)	2 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	225/234 (96%)	175 (78%)	41 (18%)	9 (4%)	2	15
All	All	563/605 (93%)	456 (81%)	85 (15%)	22 (4%)	2	15

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ARG
1	A	160	TYR
2	B	82	ILE
2	B	83	ALA
2	B	218	ASP
1	A	21	GLU
1	A	198	LEU
1	A	244	LYS
2	B	87	THR
1	A	137	GLN
1	A	243	LYS
2	B	122	ARG
2	B	221	LEU
1	A	110	GLU
1	A	142	LEU
1	A	182	LYS
1	A	215	THR
2	B	152	ALA
1	A	181	VAL
2	B	2	VAL
1	A	178	VAL
2	B	41	ILE

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	291/316 (92%)	232 (80%)	59 (20%)	1	4
2	B	197/204 (97%)	152 (77%)	45 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	488/520 (94%)	384 (79%)	104 (21%)	1 3

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	21	GLU
1	A	25	LEU
1	A	36	GLU
1	A	38	VAL
1	A	48	THR
1	A	65	GLU
1	A	78	LYS
1	A	86	THR
1	A	87	GLU
1	A	91	ILE
1	A	96	LEU
1	A	97	ARG
1	A	106	GLU
1	A	113	TYR
1	A	134	MET
1	A	139	ILE
1	A	142	LEU
1	A	149	ILE
1	A	150	ASN
1	A	151	LEU
1	A	152	LEU
1	A	155	ARG
1	A	156	LEU
1	A	157	ARG
1	A	158	GLU
1	A	160	TYR
1	A	161	SER
1	A	162	LEU
1	A	171	LEU
1	A	173	LYS
1	A	174	HIS
1	A	184	VAL
1	A	195	LEU
1	A	200	LEU
1	A	202	GLU
1	A	205	ILE

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Mol	Chain	Res	Type
1	A	209	LEU
1	A	210	GLU
1	A	215	THR
1	A	216	MET
1	A	220	MET
1	A	222	GLN
1	A	227	VAL
1	A	230	GLN
1	A	234	GLU
1	A	235	ILE
1	A	240	GLN
1	A	241	LEU
1	A	243	LYS
1	A	251	ARG
1	A	253	MET
1	A	267	LYS
1	A	275	LEU
1	A	293	LEU
1	A	313	VAL
1	A	335	LEU
1	A	345	VAL
1	A	355	GLU
2	B	16	ILE
2	B	17	ASP
2	B	18	ASP
2	B	26	THR
2	B	27	LYS
2	B	34	ARG
2	B	36	TYR
2	B	39	ARG
2	B	41	ILE
2	B	42	LYS
2	B	44	GLU
2	B	50	ILE
2	B	56	SER
2	B	58	LEU
2	B	62	ILE
2	B	68	ASN
2	B	77	VAL
2	B	78	LEU
2	B	82	ILE
2	B	87	THR

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Mol	Chain	Res	Type
2	B	91	VAL
2	B	95	VAL
2	B	104	ILE
2	B	106	PHE
2	B	109	ARG
2	B	111	LEU
2	B	117	ILE
2	B	118	VAL
2	B	135	GLU
2	B	140	LEU
2	B	141	VAL
2	B	155	THR
2	B	156	GLN
2	B	165	LYS
2	B	175	MET
2	B	181	ARG
2	B	191	GLN
2	B	198	ARG
2	B	206	VAL
2	B	207	ILE
2	B	212	LEU
2	B	217	LYS
2	B	218	ASP
2	B	221	LEU
2	B	223	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	56	ASN
1	A	174	HIS
1	A	186	HIS
1	A	230	GLN
1	A	240	GLN
1	A	291	GLN
1	A	311	HIS
2	B	7	HIS
2	B	28	ASN
2	B	64	ASN
2	B	156	GLN
2	B	219	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	A	342/371 (92%)	0.24	19 (5%) 30 23	131, 206, 298, 351	0
2	B	227/234 (97%)	0.28	10 (4%) 39 28	145, 197, 268, 338	0
All	All	569/605 (94%)	0.26	29 (5%) 33 25	131, 203, 291, 351	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	174	GLY	5.2
1	A	162	LEU	4.6
2	B	105	GLU	4.5
1	A	235	ILE	4.3
1	A	294	GLY	3.8
1	A	152	LEU	3.2
1	A	244	LYS	3.2
1	A	151	LEU	3.1
2	B	80	LEU	2.6
2	B	125	ILE	2.5
1	A	353	ILE	2.5
2	B	213	GLU	2.5
1	A	180	PHE	2.4
2	B	221	LEU	2.3
2	B	102	TYR	2.3
1	A	234	GLU	2.3
1	A	222	GLN	2.3
1	A	154	ALA	2.2
2	B	1	MET	2.2
1	A	19	PHE	2.2
1	A	216	MET	2.1
1	A	12	ASN	2.1
1	A	160	TYR	2.1
1	A	240	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	87	THR	2.1
1	A	185	GLY	2.1
1	A	326	TRP	2.0
2	B	139	ALA	2.0
1	A	233	GLU	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.