



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 03:54 AM EST

PDB ID : 3NVM
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

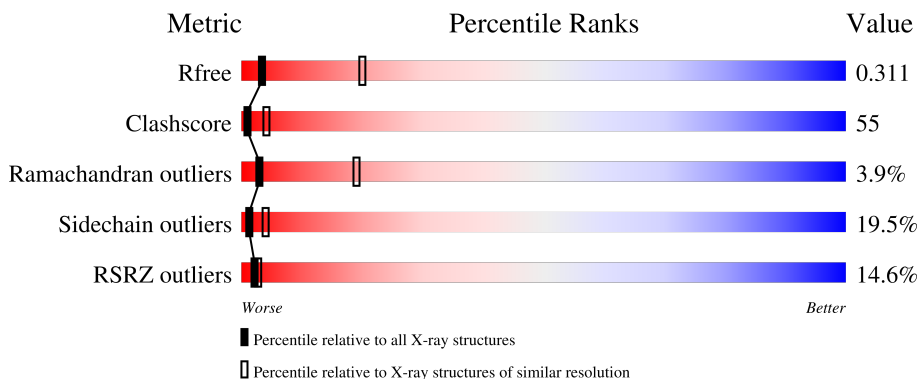
1 Overall quality at a glance

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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
2	B	234	

2 Entry composition i

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
			Total	C	N	O	S			
1	A	342	2775	1770	479	519	7	0	0	0

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 Fibrillar-like rRNA/tRNA 2'-O-methyltransferase.

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

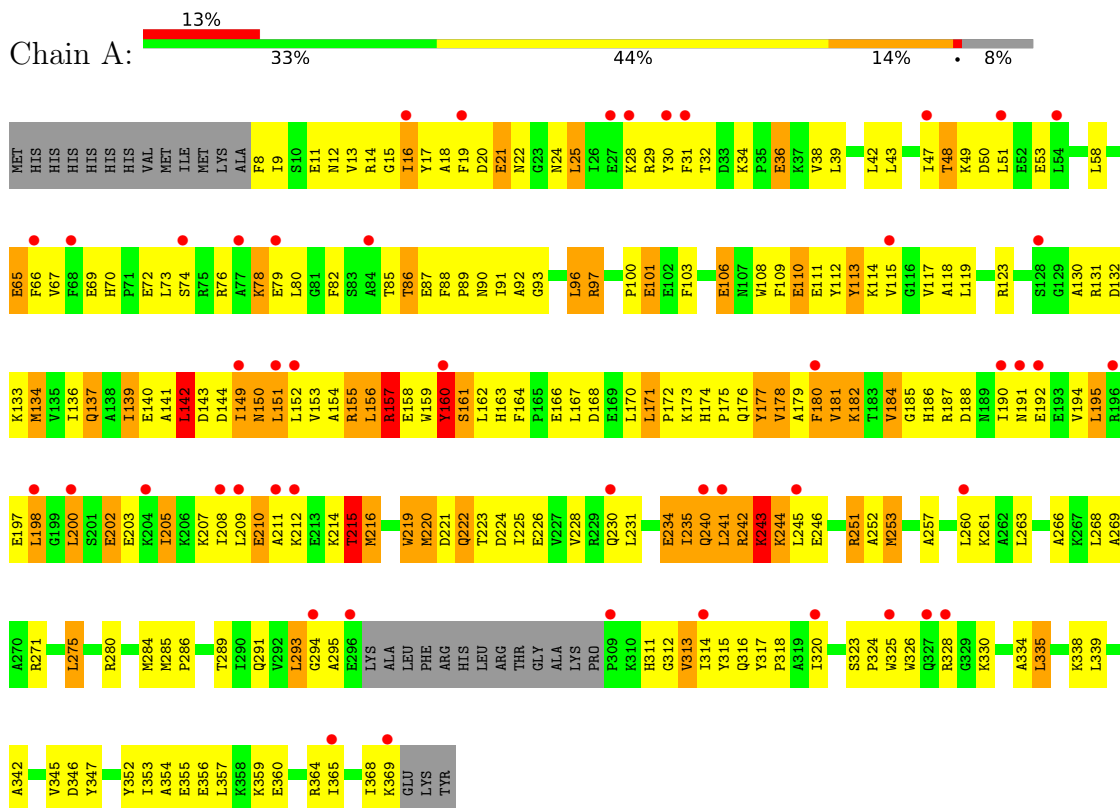
There are 7 discrepancies between the modelled and reference sequences:

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

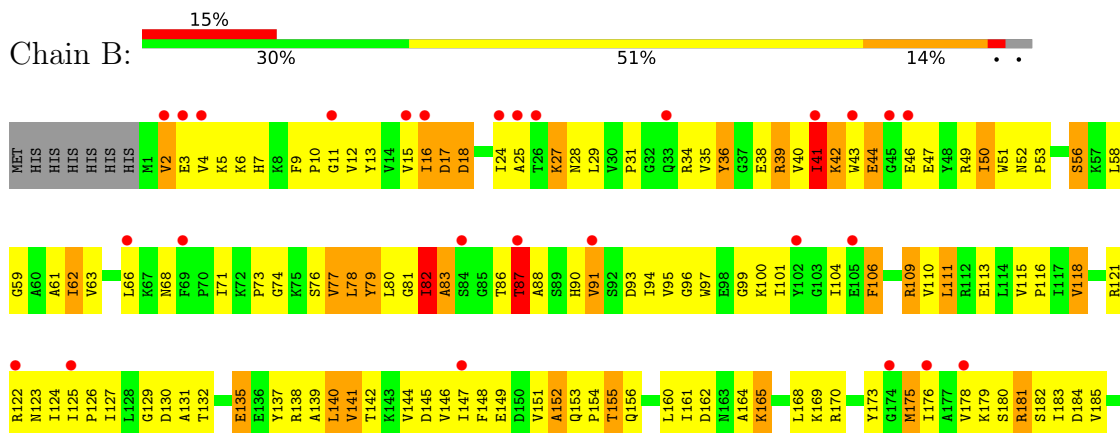
3 Residue-property plots i

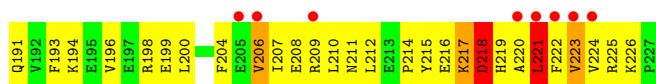
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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) 83.3 (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)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.242 , 0.316 0.242 , 0.311	Depositor DCC
R_{free} test set	907 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	126.8	Xtrriage
Anisotropy	0.452	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 180.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.063 for -h,-k,l	Xtrriage
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

Xtrriage'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	0.42	0/2824	0.60	0/3800
2	B	0.43	0/1861	0.67	1/2515 (0.0%)
All	All	0.42	0/4685	0.63	1/6315 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	221	LEU	CA-CB-CG	6.13	129.41	115.30

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	300	0
2	B	1822	0	1869	232	0
All	All	4597	0	4674	514	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 55.

All (514) 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: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: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
2:B:156:GLN:HE22	2:B:178:VAL:HA	1.44	0.82
1:A:13:VAL:HG11	1:A:111:GLU:HG2	1.62	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:159:TRP:C	1:A:161:SER:H	1.85	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:40:VAL:HG12	2:B:41:ILE:N	1.98	0.78
2:B:53:PRO:HG2	2:B:215:TYR:HE1	1.48	0.77
2:B:106:PHE:CD1	2:B:106:PHE:C	2.57	0.77
1:A:14:ARG:HG2	1:A:30:TYR:CE2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:240:GLN:NE2	1:A:240:GLN:HA	2.01	0.74
1:A:253:MET:HA	1:A:253:MET:CE	2.18	0.73
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
2:B:27:LYS:HZ1	2:B:29:LEU:HB2	1.54	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: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
2:B:106:PHE:C	2:B:106:PHE:HD1	1.95	0.70
1:A:186:HIS:HD2	1:A:188:ASP:H	1.39	0.69
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:51:TRP:HA	2:B:90:HIS:HE2	1.58	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:6:LYS:HZ1	2:B:11:GLY:N	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:240:GLN:CD	1:A:244:LYS:NZ	2.50	0.65
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
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:253:MET:HA	1:A:253:MET:HE2	1.79	0.64
1:A:119:LEU:HD11	1:A:123:ARG:NE	2.12	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
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:220:MET:CE	1:A:221:ASP:H	2.11	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:38:GLU:CD	2:B:49:ARG:HH21	2.05	0.60
1:A:156:LEU:CD1	1:A:160:TYR:HD1	2.13	0.60
2:B:27:LYS:NZ	2:B:29:LEU:HD13	2.17	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:159:TRP:C	1:A:161:SER:N	2.51	0.59
1:A:197:GLU:O	1:A:198:LEU:CB	2.50	0.59
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
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:240:GLN:CD	1:A:244:LYS:HZ3	2.06	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:6:LYS:NZ	2:B:11:GLY:N	2.52	0.57
2:B:35:VAL:O	2:B:36:TYR:CD1	2.57	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:69:GLU:CD	1:A:97:ARG:HH12	2.08	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:61:ALA:CB	2:B:221:LEU:HD23	2.35	0.57
2:B:86:THR:C	2:B:88:ALA:H	2.08	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: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
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: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:52:ASN:OD1	2:B:52:ASN:C	2.44	0.55
1:A:174:HIS:CD2	1:A:174:HIS:N	2.74	0.55
2:B:6:LYS:NZ	2:B:11:GLY:H	2.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:100:LYS:C	2:B:101:ILE:HD12	2.27	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
2:B:181:ARG:HD3	2:B:181:ARG:N	2.21	0.53
2:B:123:ASN:CG	2:B:123:ASN:O	2.47	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
2:B:27:LYS:HZ1	2:B:29:LEU:CB	2.21	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
1:A:240:GLN:HE21	1:A:244:LYS:HD3	1.73	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
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:215:TYR:C	2:B:216:GLU:HG2	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:160:TYR:C	1:A:160:TYR:CD2	2.84	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:130:ASP:OD1	2:B:132:THR:HG23	2.09	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
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:160:TYR:HD2	1:A:160:TYR:C	2.14	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:79:TYR:C	2:B:79:TYR:HD2	2.15	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
2:B:185:VAL:HG22	2:B:185:VAL:O	2.11	0.50
2:B:198:ARG:HE	2:B:199:GLU:N	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:PHE:CD1	2:B:106:PHE:O	2.65	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:177:TYR:C	1:A:179:ALA:H	2.14	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:342:ALA:O	1:A:346:ASP:HB2	2.13	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: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
2:B:79:TYR:C	2:B:79:TYR:CD2	2.86	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
2:B:36:TYR:OH	2:B:50:ILE:O	2.31	0.48
2:B:135:GLU:O	2:B:138:ARG:HG2	2.14	0.48
1:A:109:PHE:O	1:A:110:GLU:C	2.52	0.47
2:B:28:ASN:HB2	2:B:49:ARG:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:121:ARG:C	2:B:123:ASN:H	2.18	0.47
2:B:156:GLN:HG3	2:B:183:ILE:HD11	1.96	0.47
1:A:161:SER:C	1:A:164:PHE:H	2.18	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:177:TYR:C	1:A:179:ALA:N	2.68	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
1:A:178:VAL:HG13	1:A:231:LEU:HD12	1.97	0.47
2:B:123:ASN:C	2:B:124:ILE:HG13	2.35	0.47
2:B:125:ILE:HG22	2:B:127:ILE:HG13	1.96	0.47
1:A:78:LYS:C	1:A:80:LEU:H	2.17	0.46
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: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: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:139:ILE:HG22	1:A:140:GLU:N	2.31	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
1:A:251:ARG:HG3	1:A:251:ARG:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:27:LYS:HZ2	2:B:29:LEU:HD13	1.81	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:O	1:A:251:ARG:CG	2.64	0.45
2:B:88:ALA:HA	2:B:91:VAL:CG1	2.46	0.45
2:B:156:GLN:CB	2:B:176:ILE:HD11	2.46	0.45
1:A:12:ASN:OD1	1:A:17:TYR:HE1	1.98	0.45
1:A:186:HIS:CE1	1:A:219:TRP:CE3	3.02	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:155:THR:O	2:B:156:GLN:C	2.55	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
1:A:210:GLU:CD	1:A:214:LYS:HG2	2.37	0.45
2:B:179:LYS:HB3	2:B:182:SER:HB3	1.98	0.45
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
2:B:58:LEU:O	2:B:59:GLY:C	2.55	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
2:B:221:LEU:HD12	2:B:221:LEU:C	2.38	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:38:GLU:CD	2:B:49:ARG:NH2	2.71	0.44
2:B:161:ILE:O	2:B:165:LYS:CG	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:38:GLU:CD	2:B:49:ARG:HD2	2.39	0.43
1:A:113:TYR:CD2	1:A:113:TYR:C	2.91	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
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
1:A:113:TYR:O	1:A:114:LYS:C	2.57	0.43
2:B:53:PRO:HB2	2:B:215:TYR:CD1	2.53	0.43
1:A:334:ALA:O	1:A:338:LYS:HG2	2.18	0.43
2:B:217:LYS:O	2:B:219:HIS:CD2	2.72	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: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
2:B:204:PHE:CD1	2:B:224:VAL:HG11	2.54	0.42
1:A:243:LYS:O	1:A:244:LYS:C	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:B:6:LYS:HZ3	2:B:11:GLY:H	1.66	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:150:ASN:CG	1:A:151:LEU:HD13	2.41	0.41
1:A:240:GLN:HE21	1:A:240:GLN:CA	2.34	0.41
1:A:117:VAL:O	1:A:118:ALA:C	2.58	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:8:PHE:CZ	1:A:65:GLU:CD	2.95	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: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:156:GLN:HG3	2:B:183:ILE:CD1	2.51	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
1:A:156:LEU:HD13	1:A:160:TYR:CE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:82:ILE:O	2:B:83:ALA:C	2.59	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
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
1:A:221:ASP:OD2	1:A:221:ASP:C	2.60	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: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
2:B:86:THR:C	2:B:88:ALA:N	2.75	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%)	3	19
2	B	225/234 (96%)	175 (78%)	41 (18%)	9 (4%)	3	18
All	All	563/605 (93%)	456 (81%)	85 (15%)	22 (4%)	3	19

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 [i](#)

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%)	234 (80%)	57 (20%)	1 4
2	B	197/204 (97%)	159 (81%)	38 (19%)	1 4
All	All	488/520 (94%)	393 (80%)	95 (20%)	1 4

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE

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Mol	Chain	Res	Type
1	A	21	GLU
1	A	25	LEU
1	A	36	GLU
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	101	GLU
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	171	LEU
1	A	177	TYR
1	A	180	PHE
1	A	184	VAL
1	A	195	LEU
1	A	200	LEU
1	A	202	GLU
1	A	205	ILE
1	A	209	LEU
1	A	210	GLU
1	A	215	THR
1	A	216	MET
1	A	219	TRP
1	A	220	MET
1	A	222	GLN

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Mol	Chain	Res	Type
1	A	230	GLN
1	A	234	GLU
1	A	235	ILE
1	A	240	GLN
1	A	241	LEU
1	A	242	ARG
1	A	243	LYS
1	A	251	ARG
1	A	253	MET
1	A	275	LEU
1	A	293	LEU
1	A	313	VAL
1	A	335	LEU
1	A	345	VAL
2	B	16	ILE
2	B	17	ASP
2	B	18	ASP
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	62	ILE
2	B	68	ASN
2	B	77	VAL
2	B	78	LEU
2	B	79	TYR
2	B	82	ILE
2	B	87	THR
2	B	91	VAL
2	B	106	PHE
2	B	109	ARG
2	B	111	LEU
2	B	118	VAL
2	B	135	GLU
2	B	140	LEU
2	B	141	VAL
2	B	155	THR

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Mol	Chain	Res	Type
2	B	165	LYS
2	B	175	MET
2	B	181	ARG
2	B	191	GLN
2	B	206	VAL
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	163	HIS
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	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.72	48 (14%) 2 3	131, 206, 298, 351	0
2	B	227/234 (97%)	0.85	35 (15%) 2 2	145, 197, 268, 338	0
All	All	569/605 (94%)	0.77	83 (14%) 2 3	131, 203, 291, 351	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	174	GLY	8.6
1	A	208	ILE	7.7
1	A	325	TRP	5.9
1	A	296	GLU	5.2
2	B	224	VAL	5.1
1	A	209	LEU	5.1
1	A	198	LEU	5.0
1	A	152	LEU	4.6
1	A	31	PHE	4.6
1	A	51	LEU	4.5
2	B	221	LEU	4.4
1	A	84	ALA	4.4
2	B	176	ILE	4.3
1	A	241	LEU	4.3
1	A	211	ALA	4.2
2	B	25	ALA	4.2
2	B	24	ILE	4.1
1	A	66	PHE	3.8
2	B	26	THR	3.8
2	B	125	ILE	3.8
2	B	102	TYR	3.7
2	B	11	GLY	3.5
1	A	16	ILE	3.5
1	A	68	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	19	PHE	3.3
1	A	190	ILE	3.3
1	A	28	LYS	3.3
1	A	192	GLU	3.2
1	A	191	ASN	3.2
1	A	212	LYS	3.2
1	A	115	VAL	3.1
1	A	245	LEU	3.1
2	B	41	ILE	3.0
2	B	105	GLU	3.0
2	B	223	VAL	3.0
1	A	47	ILE	3.0
2	B	220	ALA	3.0
1	A	309	PRO	2.9
1	A	240	GLN	2.8
1	A	230	GLN	2.8
2	B	66	LEU	2.8
1	A	77	ALA	2.8
2	B	3	GLU	2.8
1	A	180	PHE	2.7
1	A	151	LEU	2.7
1	A	294	GLY	2.7
2	B	178	VAL	2.7
1	A	30	TYR	2.6
2	B	205	GLU	2.6
2	B	2	VAL	2.6
2	B	46	GLU	2.6
1	A	320	ILE	2.5
2	B	91	VAL	2.5
2	B	69	PHE	2.5
1	A	369	LYS	2.5
1	A	196	ARG	2.4
1	A	314	ILE	2.4
2	B	206	VAL	2.4
2	B	16	ILE	2.4
1	A	149	ILE	2.4
1	A	328	ARG	2.3
1	A	27	GLU	2.3
2	B	222	PHE	2.3
1	A	365	ILE	2.3
1	A	200	LEU	2.3
2	B	33	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	87	THR	2.3
2	B	43	TRP	2.3
1	A	160	TYR	2.2
1	A	79	GLU	2.2
2	B	45	GLY	2.2
2	B	15	VAL	2.2
2	B	147	ILE	2.2
1	A	54	LEU	2.1
2	B	84	SER	2.1
1	A	260	LEU	2.1
1	A	327	GLN	2.1
1	A	74	SER	2.1
2	B	122	ARG	2.1
2	B	4	VAL	2.1
1	A	128	SER	2.0
1	A	204	LYS	2.0
2	B	209	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.