WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 12:58 AM EDT

PDB ID	:	3AVU
Title	:	Structure of viral RNA polymerase complex 2
Authors	:	Takeshita, D.; Tomita, K.
Deposited on	:	2011-03-08
Resolution	:	2.91 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 (i) 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 (i)) were used in the production of this report:

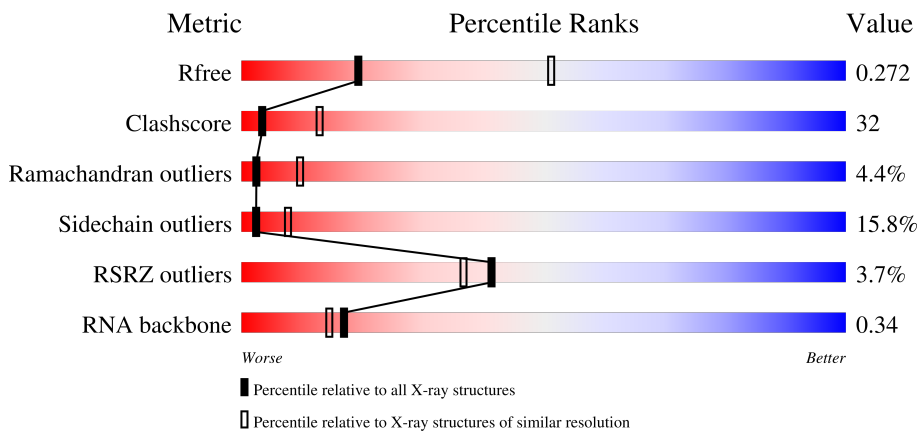|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.91 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	Percentile Ranks	Value
Rfree		0.272
Clashscore		32
Ramachandran outliers		4.4%
Sidechain outliers		15.8%
RSRZ outliers		3.7%
RNA backbone		0.34

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 <=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	1289	3% / 40% / 42% / 10% · 7%
2	G	7	29% / 43% / 57%
3	T	12	42% / 17% / 33% / 25% / 25%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 9635 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 Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1203	Total 9287	C 5865	N 1605	O 1772	S 45	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	HIS	-	linker	UNP P0A6P3
A	1284	HIS	-	expression tag	UNP Q8LTE0
A	1285	HIS	-	expression tag	UNP Q8LTE0
A	1286	HIS	-	expression tag	UNP Q8LTE0
A	1287	HIS	-	expression tag	UNP Q8LTE0
A	1288	HIS	-	expression tag	UNP Q8LTE0
A	1289	HIS	-	expression tag	UNP Q8LTE0

- Molecule 2 is a RNA chain called RNA (5'-R(*GP*GP*GP*UP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	7	Total 148	C 67	N 28	O 47	P 6	0	0	0

- Molecule 3 is a RNA chain called RNA (5'-R(*AP*UP*CP*GP*UP*GP*GP*AP*CP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	9	Total 193	C 86	N 36	O 62	P 9	8	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Ca 2	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total 4	O 4	0	0
5	T	1	Total 1	O 1	0	0

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.

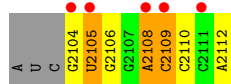• Molecule 1: Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase
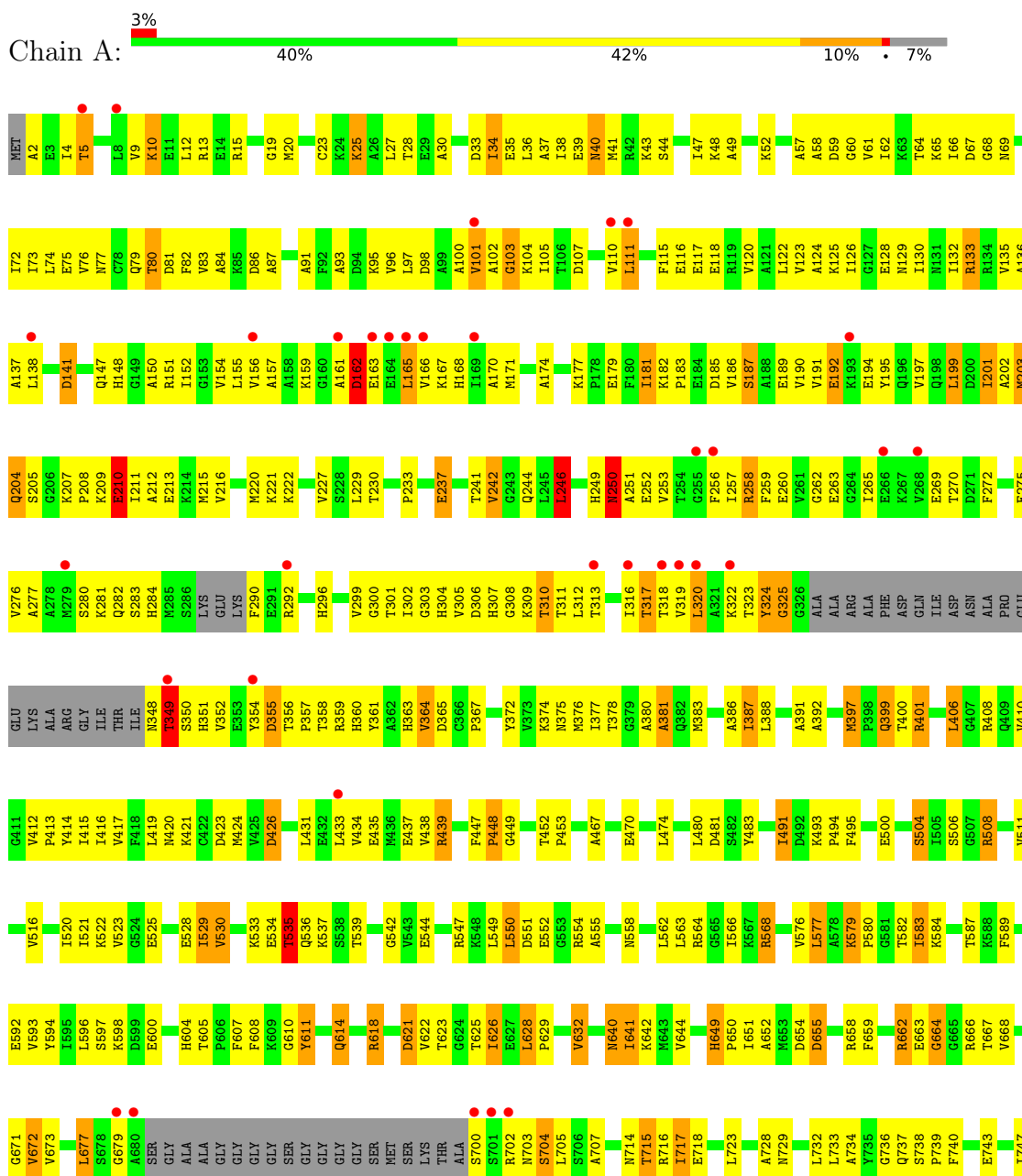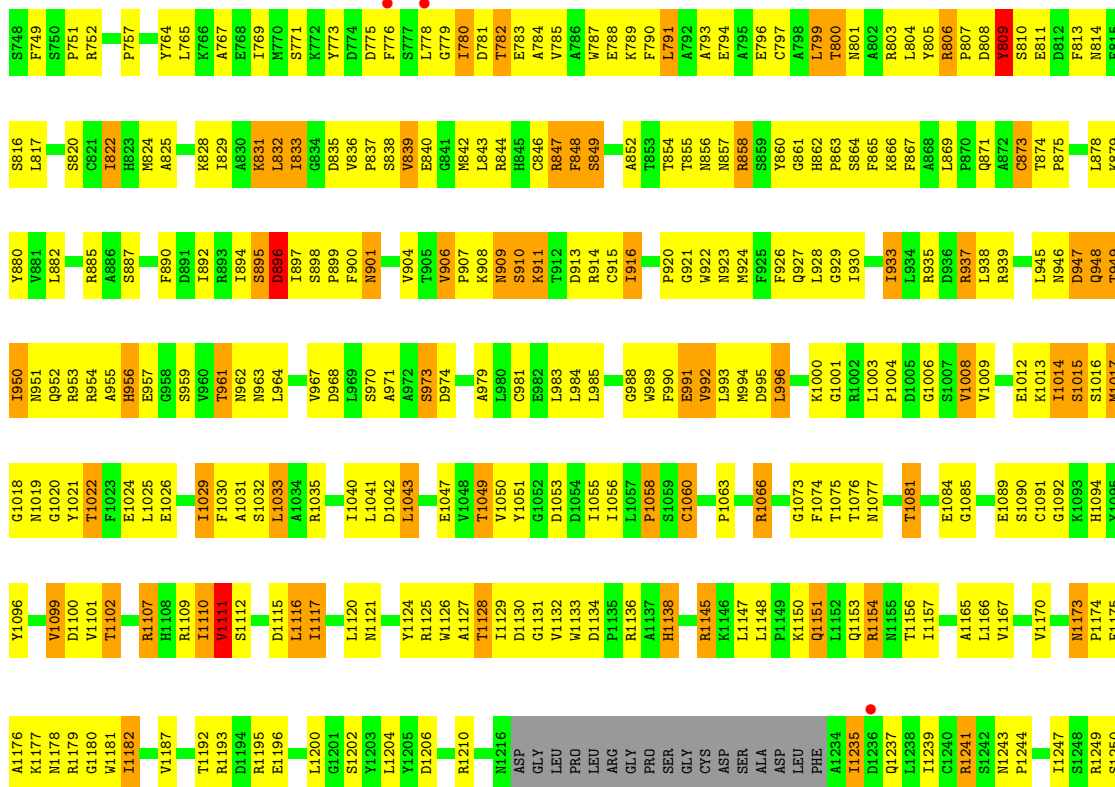
- Molecule 2: RNA (5'-R(*GP*GP*GP*UP*CP*CP*A)-3')

Chain G:
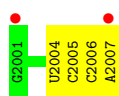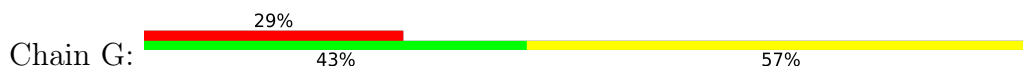
- Molecule 3: RNA (5'-R(*AP*UP*CP*GP*UP*GP*GP*AP*CP*CP*CP*A)-3')

Chain T:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	139.00Å 255.47Å 101.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.91 47.96 – 2.91	Depositor EDS
% Data completeness (in resolution range)	93.8 (19.97-2.91) 98.3 (47.96-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.219 , 0.280 0.210 , 0.272	Depositor DCC
R_{free} test set	1971 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	67.9	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 47.8	EDS
L-test for twinning [2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.028 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.030 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9635	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1/9456 (0.0%)	0.67	1/12787 (0.0%)
2	G	0.77	0/165	1.01	1/256 (0.4%)
3	T	0.65	0/215	1.05	3/333 (0.9%)
All	All	0.53	1/9836 (0.0%)	0.69	5/13376 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	981	CYS	CB-SG	-5.41	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1148	LEU	CA-CB-CG	6.28	129.74	115.30
2	G	2006	C	C6-N1-C2	-5.77	117.99	120.30
3	T	2105	U	C5-C6-N1	5.38	125.39	122.70
3	T	2105	U	C2-N1-C1'	5.35	124.12	117.70
3	T	2105	U	C6-N1-C2	-5.04	117.98	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1085	GLY	Peptide

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	A	9287	0	9273	611	0
2	G	148	0	78	7	0
3	T	193	0	99	12	0
4	A	2	0	0	0	0
5	A	4	0	0	0	0
5	T	1	0	0	0	0
All	All	9635	0	9450	615	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 32.

All (615) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:THR:HG23	1:A:953:ARG:NH1	1.58	1.17
1:A:1017:MET:HB3	2:G:2007:A:C2	1.83	1.14
1:A:949:THR:HG23	1:A:953:ARG:HH12	0.92	1.04
1:A:847:ARG:HH22	1:A:849:SER:HB2	1.24	1.02
1:A:949:THR:CG2	1:A:953:ARG:HH12	1.72	1.01
1:A:467:ALA:HA	1:A:470:GLU:HB2	1.42	1.01
1:A:1077:ASN:O	1:A:1081:THR:HG23	1.61	1.00
1:A:906:VAL:HG23	3:T:2104:G:H21	1.22	0.99
1:A:800:THR:HG22	1:A:803:ARG:HH11	1.24	0.97
1:A:212:ALA:O	1:A:216:VAL:HG23	1.67	0.94
1:A:356:THR:HG22	1:A:358:THR:H	1.30	0.94
1:A:12:LEU:HD22	1:A:27:LEU:HD13	1.49	0.93
1:A:968:ASP:H	1:A:1081:THR:HG22	1.33	0.93
1:A:304:HIS:HD2	1:A:397:MET:HG2	1.34	0.92
1:A:849:SER:HA	1:A:863:PRO:HG3	1.52	0.89
1:A:1017:MET:HB3	2:G:2007:A:H2	1.30	0.89
1:A:93:ALA:HA	1:A:96:VAL:HG12	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ARG:HH22	1:A:38:ILE:HD13	1.43	0.84
1:A:916:ILE:HD11	1:A:1017:MET:HB2	1.59	0.84
1:A:800:THR:HG22	1:A:803:ARG:NH1	1.91	0.83
1:A:10:LYS:HB3	1:A:433:LEU:HD21	1.59	0.83
1:A:356:THR:HG21	1:A:481:ASP:OD1	1.78	0.83
1:A:1047:GLU:HB3	1:A:1058:PRO:HD3	1.61	0.82
1:A:161:ALA:HB1	1:A:165:LEU:HB3	1.61	0.82
1:A:59:ASP:O	1:A:77:ASN:HB2	1.79	0.82
1:A:1003:LEU:HB3	1:A:1004:PRO:HD2	1.62	0.82
1:A:386:ALA:HB3	1:A:415:ILE:HG12	1.63	0.81
1:A:717:ILE:HD13	1:A:717:ILE:C	2.01	0.81
1:A:839:VAL:HG12	1:A:843:LEU:HD23	1.62	0.81
1:A:103:GLY:O	1:A:105:ILE:HG13	1.81	0.81
1:A:1100:ASP:OD1	1:A:1102:THR:CG2	2.29	0.80
1:A:49:ALA:HB2	1:A:123:VAL:HG11	1.63	0.80
1:A:789:LYS:HE2	1:A:789:LYS:HA	1.65	0.78
1:A:592:GLU:HG2	1:A:642:LYS:HG2	1.65	0.77
1:A:955:ALA:HB2	1:A:1090:SER:HB3	1.67	0.77
1:A:1050:VAL:HG22	1:A:1055:ILE:HA	1.67	0.77
1:A:930:ILE:HA	1:A:933:ILE:HG23	1.67	0.76
1:A:948:GLN:O	1:A:952:GLN:HG2	1.84	0.76
1:A:199:LEU:O	1:A:203:MET:HG3	1.85	0.75
1:A:1092:GLY:HA3	2:G:2005:C:H5''	1.67	0.75
1:A:604:HIS:HE1	1:A:1262:SER:HB3	1.52	0.74
1:A:847:ARG:NH2	1:A:849:SER:HB2	2.00	0.74
1:A:1019:ASN:HB3	1:A:1022:THR:HG22	1.68	0.74
1:A:148:HIS:HB3	1:A:152:ILE:CG2	2.18	0.74
1:A:805:TYR:O	1:A:806:ARG:HB2	1.85	0.74
1:A:304:HIS:CD2	1:A:397:MET:HG2	2.23	0.74
1:A:181:ILE:HG23	1:A:185:ASP:OD1	1.88	0.73
1:A:1003:LEU:HD12	1:A:1003:LEU:N	2.03	0.73
1:A:1017:MET:CB	2:G:2007:A:C2	2.66	0.73
1:A:1173:ASN:HD22	1:A:1175:PHE:H	1.36	0.73
1:A:12:LEU:HG	1:A:23:CYS:SG	2.28	0.73
1:A:388:LEU:HB3	1:A:417:VAL:HG22	1.70	0.73
1:A:930:ILE:HD11	1:A:1021:TYR:CG	2.24	0.72
1:A:378:THR:HG23	1:A:380:ALA:H	1.54	0.72
1:A:930:ILE:HD11	1:A:1021:TYR:CB	2.19	0.72
1:A:191:VAL:HG13	1:A:220:MET:HE2	1.72	0.72
1:A:596:LEU:HD12	1:A:600:GLU:HB2	1.71	0.72
1:A:504:SER:HB2	1:A:568:ARG:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ILE:O	1:A:215:MET:HG3	1.91	0.71
1:A:1096:TYR:O	1:A:1099:VAL:HG13	1.91	0.71
1:A:1100:ASP:OD1	1:A:1102:THR:HG22	1.89	0.70
1:A:1151:GLN:HE21	1:A:1151:GLN:H	1.37	0.70
1:A:375:ASN:HA	1:A:378:THR:HG22	1.73	0.70
1:A:1025:LEU:HG	1:A:1029:ILE:HD13	1.75	0.69
1:A:779:GLY:C	1:A:781:ASP:H	1.94	0.69
1:A:906:VAL:HG13	1:A:914:ARG:HB3	1.75	0.69
1:A:806:ARG:H	1:A:807:PRO:HD3	1.57	0.69
1:A:1031:ALA:O	1:A:1035:ARG:HG3	1.92	0.69
1:A:618:ARG:HG2	1:A:618:ARG:HH21	1.57	0.69
1:A:874:THR:CG2	1:A:923:ASN:HD21	2.05	0.69
1:A:237:GLU:OE2	1:A:237:GLU:HA	1.91	0.68
1:A:906:VAL:HG23	3:T:2104:G:N2	2.04	0.68
1:A:1100:ASP:OD1	1:A:1102:THR:HG23	1.93	0.68
1:A:419:LEU:HD11	1:A:434:VAL:HG11	1.76	0.68
1:A:148:HIS:HB3	1:A:152:ILE:HG22	1.76	0.67
1:A:365:ASP:O	1:A:367:PRO:HD3	1.93	0.67
1:A:833:ILE:HG23	1:A:989:TRP:CE2	2.30	0.67
1:A:380:ALA:O	1:A:381:ALA:HB2	1.95	0.67
1:A:276:VAL:HG11	1:A:352:VAL:HG11	1.75	0.67
1:A:229:LEU:HG	1:A:242:VAL:HG11	1.75	0.67
1:A:861:GLY:O	1:A:866:LYS:HE3	1.95	0.66
1:A:614:GLN:HE22	1:A:664:GLY:H	1.41	0.66
1:A:290:PHE:N	1:A:292:ARG:HH11	1.93	0.66
1:A:968:ASP:N	1:A:1081:THR:HG22	2.10	0.66
1:A:837:PRO:HG2	1:A:992:VAL:HG21	1.76	0.66
1:A:406:LEU:O	1:A:410:VAL:HG12	1.96	0.66
1:A:392:ALA:HB2	1:A:419:LEU:HD12	1.78	0.65
1:A:663:GLU:HG2	1:A:1182:ILE:HD12	1.76	0.65
1:A:1173:ASN:ND2	1:A:1175:PHE:H	1.95	0.65
1:A:187:SER:O	1:A:190:VAL:HG12	1.96	0.65
1:A:1180:GLY:O	1:A:1181:TRP:HB2	1.96	0.65
1:A:1003:LEU:HD11	1:A:1009:VAL:HG23	1.80	0.64
1:A:923:ASN:O	1:A:927:GLN:HG3	1.97	0.64
1:A:898:SER:OG	1:A:899:PRO:HD2	1.97	0.64
1:A:439:ARG:HG2	1:A:449:GLY:O	1.96	0.64
1:A:797:CYS:HB2	1:A:1012:GLU:HB3	1.79	0.63
1:A:874:THR:HA	1:A:898:SER:O	1.98	0.63
1:A:30:ALA:O	1:A:33:ASP:HB2	1.98	0.63
1:A:1195:ARG:HG2	1:A:1196:GLU:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:SER:OG	1:A:896:ASP:N	2.30	0.63
1:A:961:THR:HG22	1:A:963:ASN:H	1.63	0.62
1:A:1014:ILE:HG23	1:A:1015:SER:HB3	1.80	0.62
1:A:221:LYS:HD3	1:A:222:LYS:N	2.15	0.62
1:A:604:HIS:CE1	1:A:1262:SER:HB3	2.32	0.62
1:A:729:ASN:HD21	1:A:740:PHE:H	1.47	0.62
1:A:1117:ILE:HD13	1:A:1166:LEU:HG	1.82	0.62
1:A:133:ARG:NH2	1:A:263:GLU:O	2.32	0.62
1:A:208:PRO:HG2	1:A:211:ILE:HG13	1.81	0.62
1:A:296:HIS:CD2	1:A:360:HIS:HD2	2.17	0.62
1:A:732:LEU:HD12	1:A:739:PRO:HA	1.82	0.61
1:A:747:ILE:HG22	1:A:771:SER:HA	1.82	0.61
1:A:749:PHE:HD1	1:A:767:ALA:HB2	1.65	0.61
1:A:202:ALA:HB1	1:A:207:LYS:HD2	1.82	0.61
1:A:558:ASN:HB3	1:A:1210:ARG:HB3	1.82	0.61
1:A:302:ILE:O	1:A:388:LEU:HD12	2.01	0.61
1:A:304:HIS:CE1	1:A:305:VAL:HG12	2.35	0.61
1:A:662:ARG:HD2	1:A:667:THR:HG22	1.83	0.61
1:A:991:GLU:O	1:A:994:MET:N	2.34	0.61
1:A:96:VAL:HG21	1:A:132:ILE:CD1	2.31	0.61
1:A:65:LYS:HB2	1:A:97:LEU:CD1	2.31	0.60
1:A:828:LYS:HE2	1:A:1035:ARG:HB2	1.82	0.60
1:A:19:GLY:O	1:A:23:CYS:HB2	2.00	0.60
1:A:351:HIS:CG	1:A:351:HIS:O	2.55	0.60
1:A:808:ASP:O	1:A:809:TYR:C	2.39	0.60
1:A:892:ILE:HG23	1:A:922:TRP:CZ2	2.35	0.60
1:A:73:ILE:HD13	1:A:259:PHE:CD1	2.37	0.60
1:A:968:ASP:H	1:A:1081:THR:CG2	2.11	0.60
1:A:658:ARG:HG2	1:A:658:ARG:HH11	1.67	0.60
1:A:37:ALA:O	1:A:41:MET:HG3	2.02	0.60
1:A:871:GLN:HE21	1:A:921:GLY:HA3	1.67	0.59
1:A:1047:GLU:HB3	1:A:1058:PRO:CD	2.30	0.59
1:A:516:VAL:HG13	1:A:555:ALA:HA	1.84	0.59
1:A:874:THR:HG22	1:A:923:ASN:HD21	1.67	0.59
1:A:80:THR:HG23	1:A:82:PHE:H	1.66	0.59
1:A:589:PHE:HA	1:A:677:LEU:H	1.68	0.59
1:A:83:VAL:HG21	1:A:128:GLU:OE2	2.02	0.59
1:A:1019:ASN:HB3	1:A:1022:THR:CG2	2.32	0.59
1:A:128:GLU:O	1:A:130:ILE:HG23	2.02	0.59
1:A:839:VAL:HG12	1:A:843:LEU:CD2	2.31	0.59
1:A:530:VAL:HG22	1:A:652:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LYS:HA	1:A:230:THR:OG1	2.02	0.58
1:A:611:TYR:N	1:A:1181:TRP:HD1	2.01	0.58
1:A:1110:ILE:HD12	1:A:1111:VAL:N	2.18	0.58
1:A:300:GLY:HA3	1:A:383:MET:SD	2.43	0.58
1:A:846:CYS:SG	1:A:929:GLY:HA3	2.44	0.58
1:A:952:GLN:O	1:A:955:ALA:HB3	2.03	0.58
1:A:628:LEU:HD12	1:A:641:ILE:HD11	1.84	0.58
1:A:717:ILE:HD13	1:A:718:GLU:N	2.18	0.58
1:A:773:TYR:CE2	1:A:775:ASP:HB3	2.38	0.58
1:A:951:ASN:OD1	1:A:1049:THR:HG23	2.02	0.58
1:A:956:HIS:O	1:A:959:SER:HB3	2.04	0.58
1:A:423:ASP:OD2	1:A:424:MET:HG3	2.03	0.58
1:A:72:ILE:HD11	1:A:135:VAL:HG22	1.85	0.58
1:A:399:GLN:H	1:A:399:GLN:HE21	1.52	0.58
1:A:801:ASN:HD22	1:A:1012:GLU:HG3	1.69	0.58
1:A:111:LEU:HD23	1:A:111:LEU:H	1.68	0.58
1:A:743:GLU:HB3	1:A:776:PHE:CD2	2.39	0.58
1:A:920:PRO:O	1:A:923:ASN:HB2	2.02	0.58
1:A:152:ILE:HD11	1:A:258:ARG:CZ	2.34	0.58
1:A:262:GLY:HA2	1:A:265:ILE:HD12	1.85	0.58
1:A:467:ALA:HA	1:A:470:GLU:CB	2.28	0.58
1:A:626:ILE:HD13	1:A:626:ILE:H	1.69	0.58
1:A:299:VAL:O	1:A:364:VAL:HG23	2.04	0.58
1:A:939:ARG:HB3	1:A:939:ARG:NH1	2.19	0.58
1:A:80:THR:HG22	1:A:83:VAL:HG23	1.86	0.58
1:A:155:LEU:O	1:A:256:PHE:HA	2.04	0.57
1:A:210:GLU:OE2	1:A:210:GLU:N	2.37	0.57
1:A:1121:ASN:ND2	1:A:1167:VAL:HG23	2.19	0.57
1:A:181:ILE:CD1	1:A:253:VAL:HG23	2.34	0.57
1:A:359:ARG:NH2	1:A:480:LEU:O	2.38	0.57
1:A:824:MET:O	1:A:828:LYS:HG3	2.04	0.57
1:A:801:ASN:HA	1:A:979:ALA:HB2	1.87	0.57
1:A:49:ALA:HB2	1:A:123:VAL:CG1	2.32	0.57
1:A:65:LYS:HB2	1:A:97:LEU:HD11	1.87	0.57
1:A:152:ILE:HG13	1:A:260:GLU:HG3	1.86	0.57
1:A:177:LYS:HB3	1:A:258:ARG:CZ	2.35	0.57
1:A:939:ARG:HB3	1:A:939:ARG:HH11	1.69	0.57
1:A:846:CYS:SG	1:A:926:PHE:HA	2.44	0.57
1:A:930:ILE:HD11	1:A:1021:TYR:HB2	1.87	0.57
1:A:1173:ASN:HD22	1:A:1173:ASN:C	2.07	0.57
1:A:115:PHE:O	1:A:117:GLU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LYS:HB2	1:A:525:GLU:OE1	2.05	0.57
1:A:837:PRO:HD3	1:A:989:TRP:CD2	2.40	0.57
1:A:840:GLU:O	1:A:844:ARG:HD3	2.04	0.57
1:A:301:THR:HB	1:A:363:HIS:NE2	2.20	0.56
1:A:80:THR:HG22	1:A:83:VAL:H	1.70	0.56
1:A:500:GLU:OE1	1:A:1241:ARG:HD3	2.05	0.56
1:A:117:GLU:O	1:A:120:VAL:HG22	2.05	0.56
1:A:304:HIS:ND1	1:A:305:VAL:N	2.53	0.56
1:A:528:GLU:HG3	1:A:580:PRO:HA	1.87	0.56
1:A:528:GLU:O	1:A:577:LEU:HA	2.06	0.56
1:A:49:ALA:CB	1:A:123:VAL:HG11	2.34	0.56
1:A:154:VAL:HG21	1:A:170:ALA:O	2.05	0.56
1:A:1195:ARG:HH21	1:A:1249:ARG:HB2	1.71	0.56
1:A:316:ILE:O	1:A:320:LEU:HB2	2.04	0.56
1:A:583:ILE:HD13	1:A:584:LYS:H	1.70	0.56
1:A:900:PHE:CE2	1:A:1008:VAL:HG12	2.41	0.56
1:A:1112:SER:HB3	1:A:1115:ASP:OD1	2.05	0.56
1:A:44:SER:O	1:A:47:ILE:HG22	2.05	0.56
1:A:189:GLU:HA	1:A:192:GLU:HB2	1.88	0.56
1:A:250:ASN:HD22	1:A:251:ALA:H	1.54	0.56
1:A:324:TYR:CD1	1:A:357:PRO:HD3	2.40	0.56
1:A:658:ARG:NH1	1:A:672:VAL:HB	2.20	0.56
1:A:1053:ASP:OD1	2:G:2007:A:H4'	2.05	0.56
1:A:250:ASN:HD22	1:A:250:ASN:N	2.04	0.56
1:A:794:GLU:OE1	1:A:1013:LYS:HE2	2.05	0.56
1:A:208:PRO:HG2	1:A:211:ILE:CG1	2.36	0.56
1:A:521:ILE:O	1:A:552:GLU:HA	2.07	0.55
1:A:846:CYS:HG	1:A:926:PHE:HD1	1.54	0.55
1:A:1110:ILE:HD11	1:A:1116:LEU:HB2	1.88	0.55
1:A:61:VAL:CG1	1:A:84:ALA:HB1	2.36	0.55
1:A:990:PHE:O	1:A:994:MET:HG2	2.06	0.55
1:A:611:TYR:HB3	1:A:626:ILE:CD1	2.36	0.55
1:A:205:SER:HA	1:A:757:PRO:HG2	1.89	0.55
1:A:900:PHE:HE2	1:A:1008:VAL:HG12	1.72	0.55
1:A:194:GLU:HA	1:A:197:VAL:HG12	1.89	0.55
1:A:650:PRO:O	1:A:651:ILE:HD12	2.07	0.55
1:A:280:SER:O	1:A:284:HIS:N	2.40	0.55
1:A:312:LEU:O	1:A:316:ILE:HG13	2.07	0.55
1:A:1151:GLN:H	1:A:1151:GLN:NE2	2.04	0.55
1:A:39:GLU:O	1:A:43:LYS:HG2	2.07	0.55
1:A:130:ILE:O	1:A:130:ILE:HG13	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:HA	1:A:204:GLN:HE21	1.71	0.55
1:A:614:GLN:HE22	1:A:664:GLY:N	2.05	0.55
1:A:374:LYS:HD2	1:A:594:TYR:CE1	2.42	0.54
1:A:52:LYS:HB3	1:A:129:ASN:OD1	2.07	0.54
1:A:500:GLU:CD	1:A:1210:ARG:HH22	2.09	0.54
1:A:773:TYR:O	1:A:910:SER:HB3	2.07	0.54
1:A:837:PRO:HD3	1:A:989:TRP:CE2	2.42	0.54
1:A:930:ILE:HA	1:A:933:ILE:CG2	2.37	0.54
1:A:60:GLY:HA3	1:A:77:ASN:HA	1.89	0.54
1:A:356:THR:HG23	1:A:357:PRO:HD2	1.88	0.54
1:A:836:VAL:CG2	1:A:837:PRO:HD2	2.37	0.54
1:A:1049:THR:HG22	1:A:1056:ILE:HB	1.89	0.54
1:A:375:ASN:HA	1:A:378:THR:CG2	2.37	0.54
1:A:380:ALA:O	1:A:381:ALA:CB	2.55	0.54
1:A:951:ASN:OD1	1:A:1049:THR:CG2	2.55	0.54
1:A:871:GLN:HB2	1:A:922:TRP:CD1	2.42	0.54
1:A:1040:ILE:HG22	1:A:1040:ILE:O	2.06	0.54
1:A:62:ILE:HG12	1:A:75:GLU:HG3	1.91	0.53
1:A:351:HIS:O	1:A:351:HIS:CD2	2.62	0.53
1:A:985:LEU:HD13	1:A:993:LEU:HD22	1.89	0.53
1:A:250:ASN:N	1:A:250:ASN:ND2	2.57	0.53
1:A:544:GLU:HB3	1:A:549:LEU:HG	1.90	0.53
1:A:1151:GLN:O	1:A:1175:PHE:HE1	1.91	0.53
1:A:806:ARG:H	1:A:807:PRO:CD	2.20	0.53
1:A:67:ASP:O	1:A:69:ASN:N	2.41	0.53
1:A:529:ILE:O	1:A:529:ILE:HG12	2.06	0.53
1:A:967:VAL:HA	1:A:1081:THR:HB	1.89	0.53
1:A:5:THR:O	1:A:9:VAL:HG23	2.08	0.53
1:A:98:ASP:HA	1:A:101:VAL:HG23	1.91	0.53
1:A:181:ILE:HD13	1:A:253:VAL:HG23	1.91	0.53
1:A:420:ASN:HD22	1:A:421:LYS:HD3	1.74	0.53
1:A:1015:SER:OG	1:A:1022:THR:HB	2.09	0.53
1:A:155:LEU:N	1:A:257:ILE:O	2.41	0.53
1:A:1025:LEU:HG	1:A:1029:ILE:CD1	2.38	0.53
1:A:1170:VAL:O	1:A:1170:VAL:HG22	2.09	0.53
1:A:282:GLN:HG2	1:A:282:GLN:O	2.08	0.53
1:A:30:ALA:HB1	1:A:33:ASP:HB3	1.91	0.53
1:A:174:ALA:O	1:A:258:ARG:NH1	2.42	0.52
1:A:523:VAL:HG13	1:A:551:ASP:HA	1.92	0.52
1:A:508:ARG:HD3	1:A:562:LEU:HD21	1.90	0.52
1:A:608:PHE:HD2	1:A:1181:TRP:CZ2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:LEU:HD23	1:A:1110:ILE:HG13	1.91	0.52
1:A:773:TYR:HA	1:A:1107:ARG:O	2.09	0.52
1:A:779:GLY:C	1:A:781:ASP:N	2.62	0.52
1:A:904:VAL:CG2	1:A:916:ILE:HG22	2.39	0.52
1:A:69:ASN:HB2	1:A:141:ASP:O	2.10	0.52
1:A:152:ILE:CG1	1:A:260:GLU:HG3	2.40	0.52
1:A:899:PRO:HG2	1:A:900:PHE:CD1	2.44	0.52
1:A:1116:LEU:HD22	1:A:1120:LEU:HG	1.90	0.52
1:A:100:ALA:O	1:A:104:LYS:HA	2.09	0.52
1:A:658:ARG:HG2	1:A:658:ARG:NH1	2.24	0.52
1:A:836:VAL:HA	1:A:989:TRP:CD1	2.45	0.52
1:A:397:MET:O	1:A:400:THR:HB	2.10	0.52
1:A:48:LYS:NZ	1:A:124:ALA:HA	2.24	0.52
1:A:858:ARG:CG	3:T:2104:G:H5"	2.40	0.52
1:A:874:THR:OG1	1:A:875:PRO:HD2	2.10	0.52
1:A:195:TYR:HE1	1:A:199:LEU:HD12	1.74	0.51
1:A:491:ILE:N	1:A:491:ILE:HD13	2.24	0.51
1:A:663:GLU:O	1:A:664:GLY:O	2.27	0.51
1:A:49:ALA:O	1:A:52:LYS:HB2	2.10	0.51
1:A:190:VAL:HG13	1:A:191:VAL:HG23	1.90	0.51
1:A:714:ASN:HD21	1:A:1254:PHE:H	1.57	0.51
1:A:764:TYR:HE2	1:A:1094:HIS:CD2	2.26	0.51
1:A:947:ASP:C	1:A:949:THR:H	2.10	0.51
1:A:197:VAL:O	1:A:201:ILE:HG13	2.11	0.51
1:A:598:LYS:CD	1:A:604:HIS:HB2	2.40	0.51
1:A:971:ALA:HB1	1:A:974:ASP:HB2	1.91	0.51
1:A:1195:ARG:HD2	1:A:1247:ILE:HG21	1.93	0.51
1:A:377:ILE:HG23	1:A:671:GLY:HA2	1.91	0.51
1:A:607:PHE:CD1	1:A:611:TYR:HB2	2.46	0.51
1:A:1176:ALA:O	1:A:1178:ASN:N	2.43	0.51
1:A:1181:TRP:HA	1:A:1181:TRP:CE3	2.44	0.51
1:A:354:TYR:CE2	1:A:361:TYR:HB2	2.45	0.51
1:A:1157:ILE:HG12	1:A:1165:ALA:HB3	1.91	0.51
1:A:1173:ASN:HD21	1:A:1175:PHE:HB2	1.76	0.51
1:A:57:ALA:HA	1:A:79:GLN:HB3	1.93	0.51
1:A:704:SER:HA	1:A:707:ALA:HB3	1.93	0.51
3:T:2112:A:N3	3:T:2112:A:H2'	2.25	0.51
1:A:230:THR:HA	1:A:242:VAL:HG12	1.93	0.51
1:A:74:LEU:HD21	1:A:96:VAL:HG13	1.93	0.51
1:A:276:VAL:HG13	1:A:277:ALA:N	2.25	0.51
1:A:195:TYR:OH	1:A:213:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:HIS:HB2	1:A:650:PRO:HD2	1.93	0.51
1:A:700:SER:O	1:A:1179:ARG:HD2	2.11	0.51
1:A:828:LYS:O	1:A:831:LYS:HG3	2.11	0.51
1:A:908:LYS:HG2	1:A:909:ASN:N	2.25	0.50
1:A:947:ASP:C	1:A:949:THR:N	2.65	0.50
1:A:728:ALA:O	1:A:732:LEU:HG	2.11	0.50
1:A:901:ASN:HD22	1:A:901:ASN:H	1.58	0.50
1:A:1206:ASP:O	1:A:1210:ARG:HG3	2.11	0.50
1:A:387:ILE:HA	1:A:416:ILE:O	2.11	0.50
1:A:703:ASN:C	1:A:705:LEU:H	2.14	0.50
1:A:797:CYS:CB	1:A:1012:GLU:HB3	2.42	0.50
1:A:829:ILE:HD11	1:A:1032:SER:CB	2.42	0.50
1:A:1173:ASN:ND2	1:A:1174:PRO:HD2	2.26	0.50
1:A:195:TYR:CE1	1:A:199:LEU:HD12	2.47	0.50
1:A:1003:LEU:N	1:A:1003:LEU:CD1	2.74	0.50
1:A:306:ASP:C	1:A:308:GLY:H	2.15	0.50
1:A:310:THR:O	1:A:313:THR:HG22	2.11	0.50
1:A:191:VAL:HG12	1:A:191:VAL:O	2.10	0.50
1:A:610:GLY:H	1:A:1181:TRP:HE1	1.59	0.50
1:A:138:LEU:HD21	1:A:157:ALA:N	2.27	0.50
1:A:784:ALA:O	1:A:788:GLU:HG3	2.12	0.50
1:A:864:SER:HB2	1:A:1202:SER:HA	1.94	0.50
1:A:629:PRO:HD2	1:A:632:VAL:HG11	1.94	0.49
1:A:749:PHE:CD1	1:A:767:ALA:HB2	2.47	0.49
1:A:1032:SER:OG	1:A:1033:LEU:N	2.44	0.49
1:A:1237:GLN:O	1:A:1237:GLN:HG2	2.12	0.49
1:A:435:GLU:O	1:A:439:ARG:HB2	2.11	0.49
1:A:1026:GLU:HB2	1:A:1030:PHE:CE1	2.47	0.49
1:A:416:ILE:HD11	1:A:483:TYR:HD2	1.77	0.49
1:A:860:TYR:HA	1:A:865:PHE:CD1	2.47	0.49
1:A:946:ASN:HB3	3:T:2109:C:OP1	2.13	0.49
1:A:618:ARG:NH1	1:A:652:ALA:O	2.35	0.49
1:A:621:ASP:OD2	1:A:662:ARG:NH2	2.46	0.49
1:A:662:ARG:NH2	1:A:662:ARG:HG2	2.28	0.49
1:A:662:ARG:HG2	1:A:662:ARG:HH21	1.77	0.49
1:A:869:LEU:HD12	1:A:869:LEU:N	2.27	0.49
1:A:1121:ASN:CG	1:A:1167:VAL:HG23	2.33	0.49
1:A:663:GLU:O	1:A:664:GLY:C	2.50	0.49
1:A:787:TRP:O	1:A:790:PHE:HB3	2.13	0.49
1:A:800:THR:HG21	1:A:1073:GLY:HA2	1.94	0.49
1:A:1156:THR:HA	1:A:1166:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:H	1:A:111:LEU:CD2	2.25	0.49
1:A:376:MET:HG3	1:A:410:VAL:CG2	2.43	0.49
1:A:799:LEU:HD13	1:A:799:LEU:N	2.28	0.49
1:A:1016:SER:O	1:A:1022:THR:HG21	2.12	0.49
1:A:1130:ASP:O	1:A:1132:VAL:HG23	2.13	0.49
1:A:324:TYR:O	1:A:325:GLY:O	2.30	0.49
1:A:542:GLY:N	1:A:562:LEU:HB2	2.28	0.49
1:A:865:PHE:CZ	1:A:1247:ILE:HD13	2.48	0.49
1:A:848:PHE:HD2	1:A:867:PHE:CE1	2.31	0.49
1:A:873:CYS:HB2	1:A:922:TRP:HB2	1.94	0.49
1:A:372:TYR:HE1	1:A:410:VAL:HG21	1.76	0.48
1:A:413:PRO:HB2	1:A:414:TYR:HD1	1.78	0.48
1:A:831:LYS:HD2	1:A:831:LYS:C	2.34	0.48
1:A:871:GLN:NE2	1:A:921:GLY:HA3	2.27	0.48
1:A:937:ARG:HH21	1:A:937:ARG:HG3	1.78	0.48
1:A:534:GLU:O	1:A:536:GLN:HG3	2.13	0.48
1:A:152:ILE:HD11	1:A:258:ARG:NH1	2.28	0.48
1:A:659:PHE:O	1:A:659:PHE:CD2	2.67	0.48
1:A:878:LEU:HD11	1:A:882:LEU:HD21	1.96	0.48
1:A:906:VAL:HG22	1:A:907:PRO:O	2.13	0.48
1:A:1000:LYS:HA	1:A:1009:VAL:O	2.13	0.48
1:A:550:LEU:H	1:A:550:LEU:HD22	1.78	0.48
1:A:1001:GLY:N	1:A:1009:VAL:O	2.42	0.48
1:A:179:GLU:HB2	1:A:227:VAL:CG2	2.42	0.48
1:A:858:ARG:HB2	3:T:2104:G:OP2	2.13	0.48
1:A:323:THR:O	1:A:324:TYR:O	2.31	0.48
1:A:598:LYS:HD2	1:A:604:HIS:HB2	1.94	0.48
1:A:250:ASN:HD22	1:A:251:ALA:N	2.11	0.48
1:A:794:GLU:OE1	1:A:794:GLU:HA	2.12	0.48
1:A:1195:ARG:HG2	1:A:1196:GLU:H	1.77	0.48
1:A:547:ARG:HG2	1:A:887:SER:O	2.14	0.48
1:A:1092:GLY:CA	2:G:2005:C:H5"	2.42	0.48
1:A:1133:TRP:CE3	1:A:1138:HIS:HA	2.49	0.48
1:A:204:GLN:HA	1:A:204:GLN:NE2	2.28	0.47
1:A:495:PHE:HB3	1:A:579:LYS:HE3	1.94	0.47
1:A:12:LEU:HD23	1:A:23:CYS:O	2.14	0.47
1:A:61:VAL:HG13	1:A:84:ALA:HB1	1.96	0.47
1:A:97:LEU:O	1:A:101:VAL:HG23	2.14	0.47
1:A:470:GLU:O	1:A:474:LEU:HG	2.13	0.47
1:A:957:GLU:C	1:A:959:SER:H	2.16	0.47
1:A:516:VAL:HG13	1:A:516:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ILE:O	1:A:897:ILE:HG23	2.13	0.47
1:A:1043:LEU:HA	1:A:1043:LEU:HD13	1.26	0.47
1:A:416:ILE:HG13	1:A:453:PRO:HG2	1.96	0.47
1:A:448:PRO:O	1:A:452:THR:HB	2.15	0.47
1:A:649:HIS:CB	1:A:650:PRO:HD2	2.44	0.47
1:A:40:ASN:N	1:A:40:ASN:ND2	2.60	0.47
1:A:183:PRO:HD3	1:A:230:THR:OG1	2.15	0.47
1:A:1121:ASN:HD21	1:A:1167:VAL:H	1.62	0.47
1:A:838:SER:O	1:A:842:MET:HB2	2.15	0.47
1:A:885:ARG:HG2	1:A:885:ARG:O	2.14	0.47
1:A:973:SER:CB	1:A:1017:MET:HG3	2.45	0.47
1:A:1195:ARG:HB3	1:A:1247:ILE:HG22	1.96	0.47
1:A:93:ALA:O	1:A:97:LEU:HB2	2.14	0.47
1:A:320:LEU:HD12	1:A:355:ASP:O	2.15	0.47
1:A:628:LEU:HB3	1:A:632:VAL:HG13	1.97	0.47
1:A:764:TYR:CE2	1:A:1094:HIS:CD2	3.02	0.47
1:A:904:VAL:HG22	1:A:916:ILE:HG22	1.96	0.47
1:A:626:ILE:H	1:A:626:ILE:CD1	2.28	0.47
1:A:937:ARG:HG3	1:A:937:ARG:NH2	2.30	0.47
1:A:107:ASP:HB3	1:A:110:VAL:HG23	1.97	0.46
1:A:130:ILE:O	1:A:130:ILE:CG1	2.63	0.46
1:A:511:VAL:HB	1:A:562:LEU:HD23	1.95	0.46
1:A:534:GLU:O	1:A:535:THR:C	2.53	0.46
1:A:447:PHE:O	1:A:449:GLY:N	2.48	0.46
1:A:376:MET:HG3	1:A:410:VAL:HG23	1.98	0.46
1:A:493:LYS:HB3	1:A:494:PRO:HD2	1.97	0.46
1:A:825:ALA:O	1:A:829:ILE:HG12	2.15	0.46
1:A:829:ILE:HD11	1:A:1032:SER:HB3	1.97	0.46
1:A:775:ASP:OD2	1:A:1109:ARG:HD3	2.15	0.46
1:A:579:LYS:O	1:A:582:THR:HB	2.16	0.46
1:A:629:PRO:HD3	1:A:642:LYS:O	2.15	0.46
1:A:1235:ILE:HD13	1:A:1235:ILE:N	2.30	0.46
1:A:734:ALA:O	1:A:1136:ARG:HB3	2.16	0.46
1:A:1047:GLU:HB3	1:A:1058:PRO:CG	2.46	0.46
1:A:579:LYS:HE3	1:A:579:LYS:HB2	1.68	0.46
1:A:852:ALA:N	3:T:2105:U:H5"	2.30	0.46
1:A:1173:ASN:HD22	1:A:1174:PRO:N	2.13	0.46
1:A:34:ILE:HG22	1:A:35:GLU:N	2.31	0.46
1:A:520:ILE:HG12	1:A:554:ARG:HA	1.98	0.46
1:A:408:ARG:O	1:A:408:ARG:HD3	2.16	0.46
1:A:700:SER:O	1:A:1179:ARG:CD	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:LEU:HB3	1:A:983:LEU:HD11	1.98	0.46
1:A:836:VAL:HG23	1:A:988:GLY:C	2.37	0.46
1:A:73:ILE:HG23	1:A:259:PHE:CE1	2.51	0.45
1:A:117:GLU:OE1	1:A:117:GLU:HA	2.15	0.45
1:A:796:GLU:O	1:A:800:THR:HG23	2.15	0.45
1:A:911:LYS:HB3	1:A:911:LYS:HE3	1.55	0.45
1:A:528:GLU:HG3	1:A:580:PRO:CA	2.47	0.45
1:A:839:VAL:HA	1:A:842:MET:HB3	1.97	0.45
1:A:147:GLN:HE21	1:A:150:ALA:HA	1.81	0.45
1:A:611:TYR:HB3	1:A:626:ILE:HD12	1.99	0.45
1:A:790:PHE:HD1	1:A:791:LEU:HD13	1.81	0.45
1:A:1004:PRO:C	1:A:1006:GLY:H	2.18	0.45
1:A:1165:ALA:HB2	1:A:1187:VAL:HG12	1.98	0.45
1:A:233:PRO:HA	1:A:241:THR:HA	1.99	0.45
1:A:272:PHE:O	1:A:275:GLU:HB3	2.16	0.45
1:A:611:TYR:HB3	1:A:626:ILE:HD11	1.98	0.45
1:A:789:LYS:HA	1:A:789:LYS:CE	2.38	0.45
1:A:822:ILE:HB	1:A:984:LEU:HD11	1.98	0.45
1:A:862:HIS:CD2	1:A:864:SER:H	2.34	0.45
1:A:990:PHE:O	1:A:990:PHE:CG	2.69	0.45
1:A:1129:ILE:O	1:A:1129:ILE:HG22	2.16	0.45
1:A:1195:ARG:HD2	1:A:1247:ILE:CG2	2.46	0.45
1:A:25:LYS:O	1:A:28:THR:HG22	2.16	0.45
1:A:73:ILE:HB	1:A:155:LEU:HD22	1.98	0.45
1:A:618:ARG:HH21	1:A:618:ARG:CG	2.28	0.45
1:A:717:ILE:C	1:A:717:ILE:CD1	2.78	0.45
1:A:1090:SER:O	1:A:1091:CYS:HB2	2.16	0.45
1:A:86:ASP:CG	1:A:87:ALA:N	2.70	0.45
1:A:96:VAL:HG23	1:A:115:PHE:CE1	2.51	0.45
1:A:161:ALA:HB1	1:A:165:LEU:CB	2.41	0.45
1:A:210:GLU:HA	1:A:213:GLU:HB3	1.99	0.45
1:A:640:ASN:O	1:A:641:ILE:HB	2.17	0.45
1:A:1157:ILE:O	1:A:1167:VAL:HA	2.16	0.45
1:A:843:LEU:HD13	1:A:843:LEU:HA	1.85	0.45
1:A:1025:LEU:HA	1:A:1025:LEU:HD12	1.59	0.45
2:G:2004:U:H2'	2:G:2005:C:H5'	1.99	0.45
1:A:281:LYS:C	1:A:283:SER:H	2.20	0.45
1:A:316:ILE:O	1:A:316:ILE:HG22	2.17	0.45
1:A:361:TYR:CZ	1:A:480:LEU:HB3	2.52	0.45
1:A:1145:ARG:CD	1:A:1153:GLN:HG2	2.47	0.45
1:A:195:TYR:O	1:A:199:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:HIS:HB3	1:A:307:HIS:CG	2.51	0.45
1:A:348:ASN:O	1:A:349:THR:O	2.35	0.44
1:A:817:LEU:HD12	1:A:817:LEU:O	2.18	0.44
1:A:413:PRO:HB2	1:A:414:TYR:CD1	2.52	0.44
1:A:927:GLN:HB2	1:A:1020:GLY:HA3	1.98	0.44
3:T:2108:A:H3'	3:T:2109:C:C6	2.52	0.44
1:A:655:ASP:HA	1:A:673:VAL:HG23	1.99	0.44
1:A:782:THR:OG1	1:A:783:GLU:N	2.47	0.44
1:A:836:VAL:HG22	1:A:837:PRO:HD2	2.00	0.44
1:A:890:PHE:CG	1:A:1204:LEU:HD21	2.53	0.44
1:A:947:ASP:OD2	1:A:950:ILE:HG23	2.18	0.44
1:A:1060:CYS:O	1:A:1063:PRO:HD2	2.18	0.44
1:A:96:VAL:HG21	1:A:132:ILE:HD11	1.99	0.44
1:A:167:LYS:O	1:A:170:ALA:HB3	2.18	0.44
1:A:168:HIS:HA	1:A:171:MET:HE2	2.00	0.44
1:A:593:VAL:HG22	1:A:641:ILE:HG23	1.98	0.44
1:A:862:HIS:HD2	1:A:864:SER:H	1.64	0.44
1:A:1021:TYR:CD1	1:A:1021:TYR:C	2.91	0.44
1:A:13:ARG:NH2	1:A:437:GLU:OE2	2.51	0.44
1:A:880:TYR:OH	1:A:995:ASP:OD1	2.31	0.44
1:A:945:LEU:O	1:A:1051:TYR:HE1	2.00	0.44
1:A:991:GLU:O	1:A:992:VAL:C	2.53	0.44
1:A:1145:ARG:HD2	1:A:1153:GLN:HG2	1.99	0.44
1:A:377:ILE:CG2	1:A:671:GLY:HA2	2.47	0.44
1:A:412:VAL:HG13	1:A:412:VAL:O	2.18	0.44
1:A:28:THR:HG23	1:A:28:THR:O	2.16	0.44
1:A:72:ILE:HD12	1:A:136:ALA:O	2.17	0.44
1:A:96:VAL:O	1:A:96:VAL:HG22	2.17	0.44
1:A:316:ILE:HG21	1:A:354:TYR:CZ	2.53	0.44
1:A:629:PRO:HG2	1:A:632:VAL:CG1	2.47	0.44
1:A:909:ASN:HB3	1:A:910:SER:H	1.63	0.44
1:A:122:LEU:HD22	1:A:130:ILE:HD13	1.98	0.43
1:A:431:LEU:C	1:A:433:LEU:N	2.71	0.43
1:A:86:ASP:CG	1:A:87:ALA:H	2.21	0.43
1:A:749:PHE:HD1	1:A:767:ALA:CB	2.30	0.43
1:A:901:ASN:HD22	1:A:901:ASN:N	2.15	0.43
1:A:608:PHE:CD2	1:A:1181:TRP:CZ2	3.07	0.43
1:A:833:ILE:HD13	1:A:833:ILE:HA	1.56	0.43
1:A:848:PHE:O	1:A:849:SER:C	2.56	0.43
1:A:1243:ASN:HA	1:A:1244:PRO:HD3	1.88	0.43
1:A:74:LEU:HB3	1:A:97:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:THR:O	1:A:322:LYS:HB2	2.18	0.43
1:A:319:VAL:HG12	1:A:474:LEU:HD21	2.01	0.43
1:A:846:CYS:HG	1:A:926:PHE:HA	1.82	0.43
1:A:954:ARG:NH1	1:A:1049:THR:HB	2.34	0.43
1:A:1018:GLY:HA2	3:T:2105:U:H2'	1.99	0.43
1:A:48:LYS:HD3	1:A:124:ALA:HA	2.01	0.43
1:A:96:VAL:HG22	1:A:111:LEU:HD12	2.01	0.43
1:A:162:ASP:HB2	1:A:163:GLU:H	1.62	0.43
1:A:831:LYS:HD2	1:A:832:LEU:N	2.33	0.43
1:A:874:THR:HG22	1:A:923:ASN:ND2	2.32	0.43
1:A:80:THR:HG23	1:A:82:PHE:N	2.31	0.43
1:A:194:GLU:HA	1:A:197:VAL:CG1	2.49	0.43
1:A:793:ALA:HB1	1:A:974:ASP:O	2.19	0.43
1:A:15:ARG:NH2	1:A:38:ILE:HG21	2.33	0.43
1:A:33:ASP:HB3	1:A:36:LEU:HB3	2.01	0.43
1:A:303:GLY:H	1:A:309:LYS:NZ	2.16	0.43
1:A:539:THR:CG2	1:A:564:ARG:HD2	2.49	0.43
1:A:156:VAL:HG12	1:A:156:VAL:O	2.17	0.43
1:A:642:LYS:HE3	1:A:642:LYS:HB3	1.75	0.43
1:A:1003:LEU:HB3	1:A:1004:PRO:CD	2.40	0.43
1:A:806:ARG:N	1:A:807:PRO:CD	2.82	0.42
1:A:1134:ASP:OD1	1:A:1136:ARG:HG3	2.19	0.42
1:A:356:THR:HG21	1:A:481:ASP:CG	2.39	0.42
1:A:438:VAL:O	1:A:438:VAL:HG22	2.19	0.42
1:A:1154:ARG:HH11	1:A:1154:ARG:CB	2.32	0.42
1:A:58:ALA:HB2	1:A:265:ILE:HG21	2.01	0.42
1:A:62:ILE:O	1:A:147:GLN:NE2	2.52	0.42
1:A:72:ILE:CD1	1:A:137:ALA:HB2	2.50	0.42
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.80	0.42
1:A:715:THR:HG23	1:A:716:ARG:N	2.33	0.42
1:A:1003:LEU:HD11	1:A:1009:VAL:CG2	2.49	0.42
1:A:1192:THR:HG22	1:A:1250:SER:HA	2.02	0.42
1:A:83:VAL:HG21	1:A:128:GLU:CD	2.39	0.42
1:A:312:LEU:O	1:A:312:LEU:HG	2.19	0.42
1:A:611:TYR:O	1:A:626:ILE:HD12	2.19	0.42
1:A:723:LEU:HD23	1:A:1110:ILE:CG1	2.48	0.42
1:A:736:GLY:C	1:A:737:GLN:HG2	2.40	0.42
1:A:1040:ILE:O	1:A:1040:ILE:CG2	2.68	0.42
1:A:1124:TYR:O	1:A:1128:THR:HB	2.20	0.42
1:A:252:GLU:OE2	1:A:253:VAL:O	2.37	0.42
1:A:924:MET:O	1:A:928:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ASN:C	1:A:715:THR:O	2.56	0.42
1:A:996:LEU:HA	1:A:996:LEU:HD12	1.78	0.42
1:A:1033:LEU:HD12	1:A:1033:LEU:HA	1.76	0.42
1:A:269:GLU:HG3	1:A:270:THR:N	2.35	0.42
1:A:307:HIS:CD2	1:A:391:ALA:H	2.37	0.42
1:A:596:LEU:HB2	1:A:668:VAL:O	2.20	0.42
1:A:9:VAL:HG12	1:A:20:MET:HE1	2.02	0.42
1:A:40:ASN:N	1:A:40:ASN:HD22	2.17	0.42
1:A:618:ARG:HG2	1:A:618:ARG:NH2	2.29	0.42
1:A:118:GLU:O	1:A:122:LEU:HB2	2.19	0.41
1:A:187:SER:HB3	1:A:190:VAL:HG12	2.02	0.41
1:A:419:LEU:HD11	1:A:434:VAL:CG1	2.46	0.41
1:A:985:LEU:CD1	1:A:993:LEU:HD22	2.50	0.41
1:A:1066:ARG:HH21	1:A:1066:ARG:CG	2.33	0.41
1:A:249:HIS:O	1:A:250:ASN:CB	2.68	0.41
1:A:452:THR:HG23	1:A:452:THR:O	2.19	0.41
1:A:626:ILE:HA	1:A:644:VAL:O	2.20	0.41
1:A:857:ASN:O	1:A:860:TYR:N	2.53	0.41
1:A:927:GLN:OE1	1:A:1020:GLY:N	2.47	0.41
1:A:1126:TRP:CE3	1:A:1127:ALA:HB2	2.56	0.41
3:T:2108:A:H5'	3:T:2109:C:OP2	2.20	0.41
1:A:120:VAL:HA	1:A:123:VAL:HG12	2.01	0.41
1:A:401:ARG:HE	1:A:401:ARG:HB3	1.50	0.41
1:A:790:PHE:CD1	1:A:791:LEU:HD13	2.54	0.41
1:A:1047:GLU:CB	1:A:1058:PRO:CG	2.99	0.41
1:A:1099:VAL:O	1:A:1101:VAL:HG13	2.20	0.41
1:A:1154:ARG:HB2	1:A:1154:ARG:NH1	2.35	0.41
1:A:1193:ARG:HD2	1:A:1249:ARG:HH12	1.85	0.41
1:A:122:LEU:O	1:A:125:LYS:N	2.53	0.41
1:A:2:ALA:N	1:A:426:ASP:O	2.53	0.41
1:A:626:ILE:HD13	1:A:626:ILE:O	2.20	0.41
1:A:935:ARG:NH2	1:A:1024:GLU:OE2	2.53	0.41
1:A:1151:GLN:HE21	1:A:1151:GLN:N	2.12	0.41
1:A:91:ALA:O	1:A:95:LYS:HB2	2.20	0.41
1:A:155:LEU:O	1:A:257:ILE:N	2.51	0.41
1:A:378:THR:CG2	1:A:380:ALA:H	2.27	0.41
1:A:1018:GLY:HA2	3:T:2105:U:C2'	2.51	0.41
1:A:64:THR:HA	1:A:72:ILE:O	2.21	0.41
1:A:126:ILE:HG23	1:A:399:GLN:HE22	1.86	0.41
1:A:229:LEU:HD11	1:A:242:VAL:HG21	2.02	0.41
1:A:281:LYS:C	1:A:283:SER:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:LEU:HA	1:A:677:LEU:HD23	1.79	0.41
1:A:810:SER:C	1:A:811:GLU:HG2	2.40	0.41
1:A:1041:LEU:C	1:A:1043:LEU:H	2.23	0.41
1:A:1254:PHE:CD1	1:A:1254:PHE:N	2.89	0.41
1:A:301:THR:HG23	1:A:365:ASP:OD2	2.20	0.41
1:A:310:THR:C	1:A:313:THR:HG22	2.41	0.41
1:A:751:PRO:HG3	1:A:767:ALA:CB	2.50	0.41
1:A:790:PHE:HB2	1:A:915:CYS:SG	2.61	0.41
1:A:916:ILE:HG12	3:T:2105:U:C2	2.55	0.41
1:A:930:ILE:CD1	1:A:1021:TYR:HB2	2.51	0.41
1:A:961:THR:CG2	1:A:963:ASN:H	2.29	0.41
1:A:4:ILE:HG22	1:A:5:THR:N	2.34	0.40
1:A:310:THR:HA	1:A:313:THR:HG22	2.02	0.40
1:A:930:ILE:CD1	1:A:1021:TYR:CB	2.94	0.40
1:A:1100:ASP:OD1	1:A:1100:ASP:C	2.59	0.40
1:A:126:ILE:HG23	1:A:399:GLN:NE2	2.37	0.40
1:A:765:LEU:O	1:A:769:ILE:HG22	2.22	0.40
1:A:856:ASN:ND2	1:A:866:LYS:HD3	2.36	0.40
1:A:938:LEU:HD12	1:A:938:LEU:HA	1.75	0.40
1:A:317:THR:HG22	1:A:354:TYR:HB3	2.03	0.40
1:A:323:THR:HG22	1:A:324:TYR:N	2.36	0.40
1:A:1204:LEU:HA	1:A:1204:LEU:HD23	1.72	0.40
1:A:1110:ILE:HD12	1:A:1111:VAL:H	1.87	0.40
1:A:1121:ASN:O	1:A:1125:ARG:HG3	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	A	1193/1289 (93%)	987 (83%)	154 (13%)	52 (4%)	2	10

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	101	VAL
1	A	116	GLU
1	A	141	ASP
1	A	209	LYS
1	A	250	ASN
1	A	324	TYR
1	A	325	GLY
1	A	349	THR
1	A	381	ALA
1	A	778	LEU
1	A	806	ARG
1	A	809	TYR
1	A	896	ASP
1	A	970	SER
1	A	1177	LYS
1	A	68	GLY
1	A	102	ALA
1	A	159	LYS
1	A	210	GLU
1	A	664	GLY
1	A	677	LEU
1	A	813	PHE
1	A	849	SER
1	A	895	SER
1	A	947	ASP
1	A	1015	SER
1	A	1074	PHE
1	A	162	ASP
1	A	577	LEU
1	A	679	GLY
1	A	1084	GLU
1	A	1241	ARG
1	A	187	SER
1	A	246	LEU
1	A	350	SER
1	A	506	SER
1	A	535	THR
1	A	611	TYR
1	A	641	ILE
1	A	702	ARG
1	A	909	ASN

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Mol	Chain	Res	Type
1	A	448	PRO
1	A	780	ILE
1	A	576	VAL
1	A	1131	GLY
1	A	103	GLY
1	A	201	ILE
1	A	566	ILE
1	A	1239	ILE
1	A	1058	PRO
1	A	1111	VAL

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	995/1060 (94%)	838 (84%)	157 (16%)	2	8

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	10	LYS
1	A	25	LYS
1	A	40	ASN
1	A	66	ILE
1	A	76	VAL
1	A	80	THR
1	A	81	ASP
1	A	111	LEU
1	A	133	ARG
1	A	151	ARG
1	A	162	ASP
1	A	165	LEU
1	A	166	VAL
1	A	181	ILE
1	A	186	VAL

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Mol	Chain	Res	Type
1	A	192	GLU
1	A	199	LEU
1	A	203	MET
1	A	204	GLN
1	A	210	GLU
1	A	237	GLU
1	A	242	VAL
1	A	244	GLN
1	A	246	LEU
1	A	250	ASN
1	A	258	ARG
1	A	310	THR
1	A	311	THR
1	A	317	THR
1	A	320	LEU
1	A	349	THR
1	A	355	ASP
1	A	364	VAL
1	A	387	ILE
1	A	397	MET
1	A	399	GLN
1	A	401	ARG
1	A	406	LEU
1	A	426	ASP
1	A	439	ARG
1	A	491	ILE
1	A	504	SER
1	A	508	ARG
1	A	529	ILE
1	A	530	VAL
1	A	533	LYS
1	A	535	THR
1	A	537	LYS
1	A	550	LEU
1	A	563	LEU
1	A	568	ARG
1	A	579	LYS
1	A	583	ILE
1	A	587	THR
1	A	597	SER
1	A	605	THR
1	A	614	GLN

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Mol	Chain	Res	Type
1	A	618	ARG
1	A	621	ASP
1	A	622	VAL
1	A	623	THR
1	A	625	THR
1	A	626	ILE
1	A	628	LEU
1	A	632	VAL
1	A	640	ASN
1	A	649	HIS
1	A	654	ASP
1	A	655	ASP
1	A	662	ARG
1	A	666	ARG
1	A	672	VAL
1	A	704	SER
1	A	715	THR
1	A	717	ILE
1	A	733	LEU
1	A	738	SER
1	A	752	ARG
1	A	780	ILE
1	A	782	THR
1	A	785	VAL
1	A	791	LEU
1	A	799	LEU
1	A	800	THR
1	A	809	TYR
1	A	814	ASN
1	A	816	SER
1	A	820	SER
1	A	822	ILE
1	A	831	LYS
1	A	832	LEU
1	A	833	ILE
1	A	835	ASP
1	A	839	VAL
1	A	847	ARG
1	A	848	PHE
1	A	854	THR
1	A	855	THR
1	A	858	ARG

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Mol	Chain	Res	Type
1	A	873	CYS
1	A	879	LYS
1	A	894	ILE
1	A	896	ASP
1	A	901	ASN
1	A	906	VAL
1	A	910	SER
1	A	911	LYS
1	A	913	ASP
1	A	916	ILE
1	A	933	ILE
1	A	937	ARG
1	A	948	GLN
1	A	949	THR
1	A	950	ILE
1	A	956	HIS
1	A	961	THR
1	A	962	ASN
1	A	964	LEU
1	A	973	SER
1	A	991	GLU
1	A	992	VAL
1	A	996	LEU
1	A	1008	VAL
1	A	1014	ILE
1	A	1017	MET
1	A	1022	THR
1	A	1029	ILE
1	A	1033	LEU
1	A	1042	ASP
1	A	1043	LEU
1	A	1049	THR
1	A	1060	CYS
1	A	1066	ARG
1	A	1075	THR
1	A	1076	THR
1	A	1081	THR
1	A	1089	GLU
1	A	1099	VAL
1	A	1102	THR
1	A	1107	ARG
1	A	1110	ILE

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Mol	Chain	Res	Type
1	A	1111	VAL
1	A	1116	LEU
1	A	1117	ILE
1	A	1128	THR
1	A	1138	HIS
1	A	1145	ARG
1	A	1147	LEU
1	A	1150	LYS
1	A	1151	GLN
1	A	1154	ARG
1	A	1173	ASN
1	A	1182	ILE
1	A	1200	LEU
1	A	1235	ILE
1	A	1251	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	114	GLN
1	A	147	GLN
1	A	168	HIS
1	A	204	GLN
1	A	250	ASN
1	A	296	HIS
1	A	307	HIS
1	A	351	HIS
1	A	360	HIS
1	A	382	GLN
1	A	399	GLN
1	A	409	GLN
1	A	420	ASN
1	A	614	GLN
1	A	714	ASN
1	A	729	ASN
1	A	763	ASN
1	A	856	ASN
1	A	862	HIS
1	A	871	GLN
1	A	901	ASN
1	A	1077	ASN

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Mol	Chain	Res	Type
1	A	1094	HIS
1	A	1121	ASN
1	A	1122	ASN
1	A	1151	GLN
1	A	1155	ASN
1	A	1173	ASN
1	A	1237	GLN
1	A	1257	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	6/7 (85%)	0	0
3	T	8/12 (66%)	4 (50%)	0
All	All	14/19 (73%)	4 (28%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	2106	G
3	T	2108	A
3	T	2109	C
3	T	2110	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7　Other polymers　ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues　ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	1203/1289 (93%)	0.15	38 (3%)	47	43	31, 80, 128, 147	0
2	G	7/7 (100%)	1.96	2 (28%)	0	0	116, 131, 163, 165	0
3	T	9/12 (75%)	2.86	5 (55%)	0	0	97, 126, 154, 160	1 (11%)
All	All	1219/1308 (93%)	0.18	45 (3%)	41	37	31, 80, 129, 165	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	701	SER	10.4
1	A	700	SER	7.6
1	A	680	ALA	6.5
3	T	2104	G	6.2
3	T	2105	U	6.2
1	A	161	ALA	5.8
1	A	320	LEU	4.8
1	A	169	ILE	4.7
2	G	2007	A	4.7
1	A	163	GLU	4.0
1	A	1236	ASP	3.3
1	A	322	LYS	3.1
1	A	319	VAL	2.9
1	A	5	THR	2.8
1	A	313	THR	2.8
1	A	156	VAL	2.8
1	A	354	TYR	2.8
1	A	318	THR	2.8
3	T	2111	C	2.7
1	A	279	MET	2.7
1	A	266	GLU	2.6
1	A	101	VAL	2.6
1	A	111	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	193	LYS	2.5
1	A	702	ARG	2.5
1	A	110	VAL	2.5
2	G	2001	G	2.5
1	A	165	LEU	2.5
3	T	2109	C	2.5
1	A	776	PHE	2.4
1	A	1263	SER	2.4
1	A	433	LEU	2.4
1	A	8	LEU	2.4
1	A	256	PHE	2.3
1	A	164	GLU	2.3
1	A	316	ILE	2.3
1	A	268	VAL	2.3
1	A	138	LEU	2.2
1	A	778	LEU	2.2
1	A	255	GLY	2.2
1	A	292	ARG	2.2
1	A	349	THR	2.2
1	A	166	VAL	2.1
1	A	679	GLY	2.0
3	T	2108	A	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	3001	1/1	0.93	0.19	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	3002	1/1	0.98	0.19	77,77,77,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.