Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 11:12 PM EDT

PDB ID	:	4ZT9
Title	:	Nuclease-inactive Streptococcus pyogenes Cas9 (D10A/H840A, dCas9) in complex with single-guide RNA at 3.1 Angstrom resolution
Authors	:	Jiang, F.; Doudna, J.A.
Deposited on	:	2015-05-14
Resolution	:	3.10 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 (1)) were used in the production of this report:

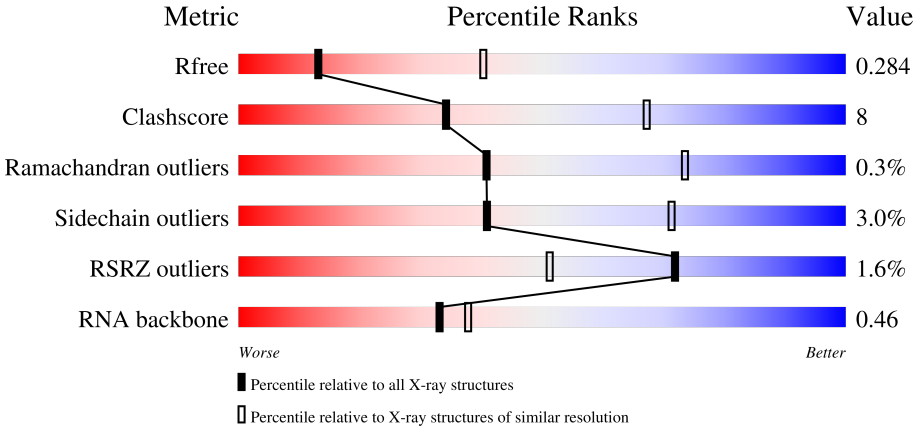
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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	1369	3% 75% 21% • •
1	C	1369	67% 17% • 15%
2	B	85	41% 38% 6% 15%
2	D	85	45% 33% 7% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 22278 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 CRISPR-associated endonuclease Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1335	10208	6499	1738	1952	19	0	0	0
1	C	1160	8980	5725	1550	1689	16	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A0C6FZC2
A	10	ALA	ASP	engineered mutation	UNP A0A0C6FZC2
A	840	ALA	HIS	engineered mutation	UNP A0A0C6FZC2
C	0	SER	-	expression tag	UNP A0A0C6FZC2
C	10	ALA	ASP	engineered mutation	UNP A0A0C6FZC2
C	840	ALA	HIS	engineered mutation	UNP A0A0C6FZC2

- Molecule 2 is a RNA chain called single-guide RNA.

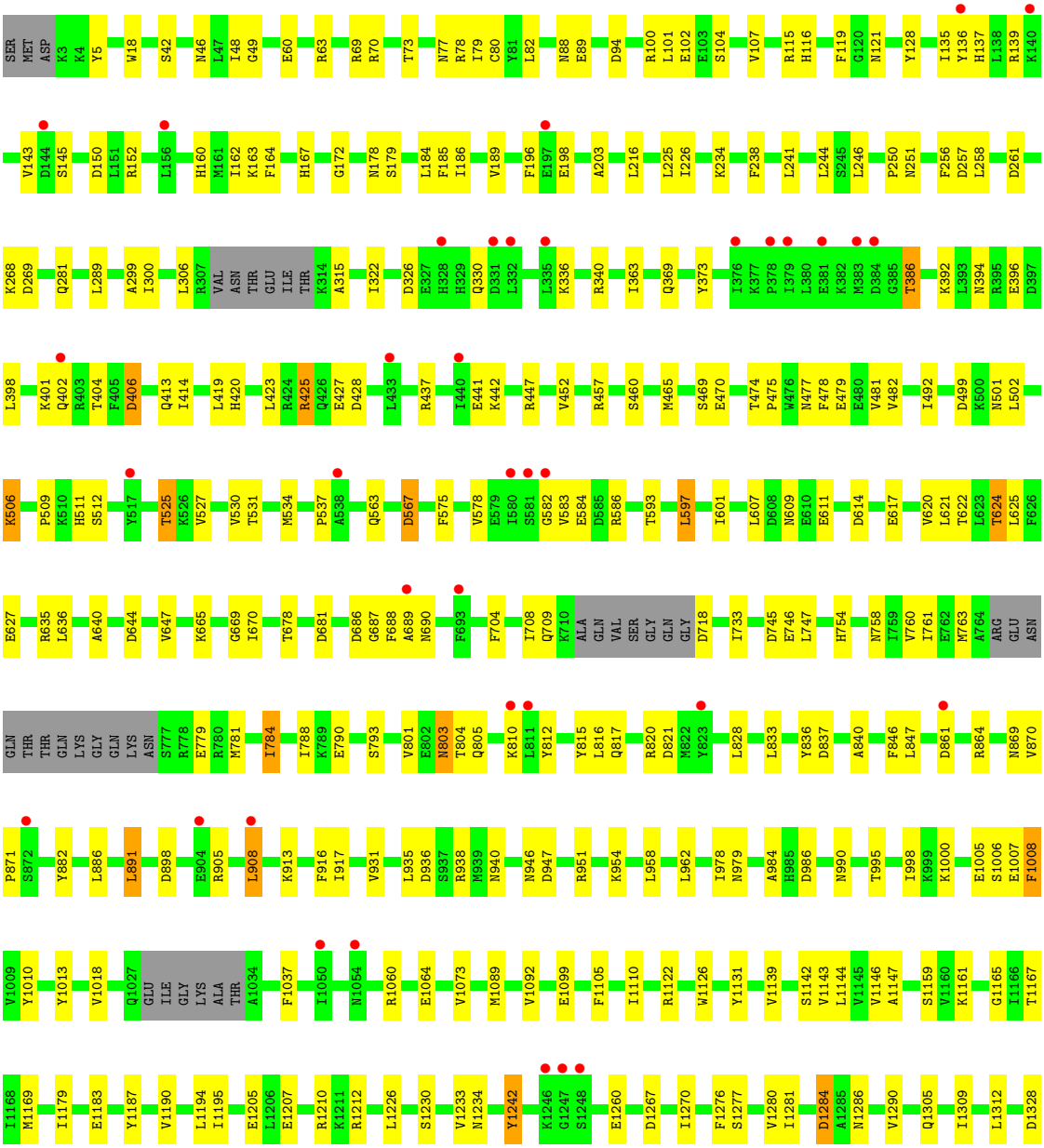
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	72	1545	692	285	496	72	0	0	0
2	D	72	1545	692	285	496	72	0	0	0

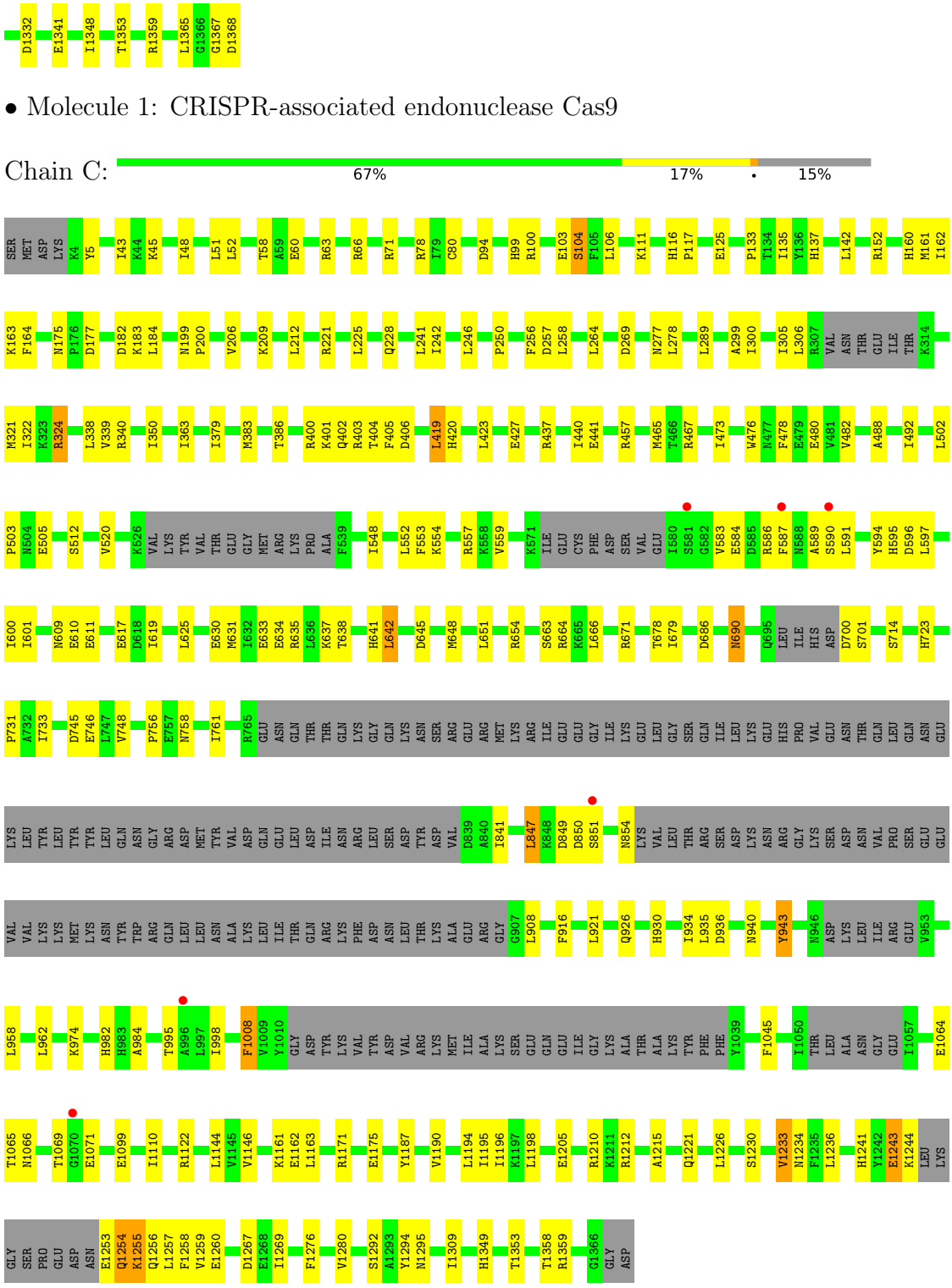
3 Residue-property plots (i)

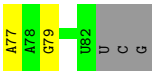
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CRISPR-associated endonuclease Cas9

Chain A:

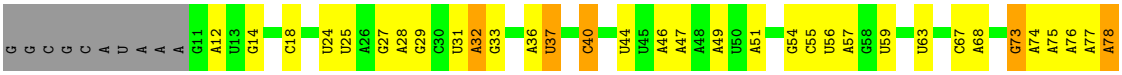


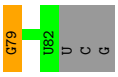

D1332 E1341 I1348 T1353 R1359 L1365 G1366 G1367 D1368
• Molecule 1: CRISPR-associated endonuclease Cas9
Chain C:
67%
17%
15%
• Molecule 2: single-guide RNA
Chain B:
41%
38%
6%
15%



• Molecule 2: single-guide RNA

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.50Å 143.05Å 296.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 3.10 148.07 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.36-3.10) 96.2 (148.07-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.97 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.243 , 0.284 0.246 , 0.284	Depositor DCC
R_{free} test set	3873 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	64.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 31.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	22278	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (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	0.37	0/10393	0.47	0/14104
1	C	0.49	1/9136 (0.0%)	0.49	0/12364
2	B	0.69	0/1732	0.87	0/2698
2	D	0.88	0/1732	0.93	3/2698 (0.1%)
All	All	0.50	1/22993 (0.0%)	0.57	3/31864 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	80	CYS	CB-SG	-23.75	1.41	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	14	G	C4-N9-C1'	6.61	135.10	126.50
2	D	14	G	O4'-C1'-N9	5.63	112.70	108.20
2	D	14	G	C8-N9-C1'	-5.32	120.09	127.00

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	10208	0	9648	183	0
1	C	8980	0	8681	157	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1545	0	774	23	0
2	D	1545	0	774	19	0
All	All	22278	0	19877	355	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 8.

All (355) 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:C:161:MET:HE1	1:C:419:LEU:HA	1.23	1.13
1:C:161:MET:HE3	1:C:419:LEU:HB2	1.33	1.10
1:C:161:MET:CE	1:C:419:LEU:HB2	1.91	0.98
1:C:161:MET:HE1	1:C:419:LEU:CA	1.96	0.96
1:C:161:MET:CE	1:C:419:LEU:CB	2.50	0.90
1:C:161:MET:CE	1:C:419:LEU:CA	2.49	0.89
1:C:161:MET:CE	1:C:419:LEU:HA	2.04	0.86
1:C:161:MET:HE3	1:C:419:LEU:CB	2.06	0.85
1:A:746:GLU:OE2	1:A:1353:THR:OG1	1.95	0.84
1:C:161:MET:HE2	1:C:419:LEU:HD12	1.61	0.83
1:C:321:MET:SD	1:C:324:ARG:NH1	2.52	0.82
1:C:1236:LEU:HD21	1:C:1309:ILE:HD11	1.61	0.82
1:C:78:ARG:NH1	1:C:162:ILE:O	2.12	0.82
1:C:182:ASP:HB3	1:C:209:LYS:HB2	1.63	0.79
1:C:100:ARG:NH1	1:C:117:PRO:O	2.16	0.78
1:C:338:LEU:HD13	1:C:386:THR:HG22	1.63	0.78
1:C:420:HIS:ND1	1:C:441:GLU:OE2	2.18	0.77
1:C:520:VAL:HG21	1:C:591:LEU:HG	1.67	0.77
1:A:761:ILE:HD11	1:A:935:LEU:HD12	1.65	0.76
2:B:73:G:H21	2:B:76:A:H2	1.30	0.76
1:A:525:THR:OG1	1:A:690:ASN:ND2	2.17	0.76
1:C:847:LEU:HD12	1:C:849:ASP:HB2	1.66	0.76
1:A:1242:TYR:OH	1:A:1260:GLU:OE2	2.06	0.72
1:C:1258:PHE:O	1:C:1260:GLU:N	2.22	0.72
1:C:761:ILE:HD11	1:C:935:LEU:HD12	1.70	0.72
1:A:189:VAL:HG21	1:A:203:ALA:HB2	1.71	0.72
1:A:1290:VAL:HG21	1:A:1312:LEU:HD13	1.72	0.72
1:A:78:ARG:NH1	1:A:162:ILE:O	2.22	0.71
1:A:340:ARG:HH12	2:B:40:C:H5"	1.56	0.71
1:A:150:ASP:OD2	1:A:152:ARG:NH1	2.24	0.70
1:A:687:GLY:O	1:A:689:ALA:N	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:HIS:CD2	2:B:46:A:H5"	2.25	0.70
1:C:256:PHE:O	1:C:258:LEU:N	2.25	0.70
1:C:1205:GLU:OE1	1:C:1359:ARG:NH2	2.25	0.70
2:D:33:G:N2	2:D:36:A:OP2	2.22	0.68
1:A:420:HIS:ND1	1:A:441:GLU:OE2	2.28	0.67
1:C:212:LEU:O	1:C:221:ARG:NE	2.27	0.67
2:D:73:G:H21	2:D:76:A:H2	1.40	0.67
2:B:42:A:O2'	2:B:43:G:OP1	2.12	0.66
1:C:553:PHE:HB3	1:C:591:LEU:HD12	1.77	0.66
1:A:402:GLN:OE1	2:B:44:U:O2'	2.14	0.66
1:A:256:PHE:O	1:A:258:LEU:N	2.28	0.66
1:A:119:PHE:HE2	1:A:128:TYR:HB2	1.61	0.66
1:A:94:ASP:OD2	1:A:100:ARG:NH1	2.30	0.65
1:C:1066:ASN:OD1	1:C:1069:THR:OG1	2.15	0.65
1:C:1230:SER:O	1:C:1234:ASN:ND2	2.30	0.65
1:C:340:ARG:NH2	2:D:40:C:OP1	2.30	0.64
1:A:530:VAL:HB	1:A:537:PRO:HB3	1.79	0.63
1:A:817:GLN:O	1:A:882:TYR:OH	2.16	0.63
1:A:1210:ARG:NH2	1:A:1341:GLU:OE2	2.30	0.63
1:C:1122:ARG:NH2	2:D:49:A:N3	2.46	0.63
1:A:160:HIS:NE2	2:B:46:A:OP1	2.28	0.63
1:C:137:HIS:HA	1:C:322:ILE:HD11	1.79	0.63
1:A:82:LEU:HD22	1:A:162:ILE:HD12	1.80	0.62
1:C:94:ASP:OD2	1:C:152:ARG:NH1	2.31	0.62
1:C:958:LEU:HD22	1:C:962:LEU:HD12	1.80	0.62
1:A:116:HIS:NE2	2:B:27:G:OP1	2.28	0.62
1:A:442:LYS:NZ	1:A:475:PRO:O	2.32	0.62
1:A:601:ILE:HA	1:A:647:VAL:HG21	1.80	0.62
1:A:474:THR:OG1	1:A:477:ASN:OD1	2.16	0.62
1:C:402:GLN:OE1	2:D:44:U:O2'	2.17	0.62
1:C:841:ILE:HD13	1:C:854:ASN:HB2	1.82	0.62
1:A:1205:GLU:OE1	1:A:1359:ARG:NH2	2.32	0.62
2:D:32:A:H61	2:D:37:U:H3	1.48	0.62
1:C:400:ARG:NH2	1:C:406:ASP:OD2	2.27	0.62
1:C:1212:ARG:NH2	1:C:1280:VAL:O	2.33	0.61
1:A:810:LYS:NZ	1:A:833:LEU:O	2.21	0.61
1:C:1146:VAL:HG12	1:C:1161:LYS:HG3	1.82	0.61
1:C:116:HIS:HB3	1:C:125:GLU:HG3	1.81	0.61
1:C:161:MET:HE3	1:C:419:LEU:CA	2.26	0.61
1:C:1253:GLU:O	1:C:1255:LYS:N	2.28	0.61
1:A:251:ASN:HD21	1:A:261:ASP:HB2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1267:ASP:OD1	1:C:1294:TYR:OH	2.15	0.61
1:C:175:ASN:ND2	1:C:177:ASP:HB2	2.16	0.60
1:C:663:SER:OG	1:C:664:ARG:N	2.32	0.60
1:C:161:MET:HE2	1:C:419:LEU:CD1	2.31	0.60
1:A:492:ILE:HG12	1:A:625:LEU:HD23	1.82	0.60
1:A:101:LEU:O	1:A:104:SER:OG	2.14	0.59
1:A:998:ILE:HD11	1:A:1005:GLU:HG2	1.83	0.59
1:A:1207:GLU:OE1	1:A:1210:ARG:NH1	2.35	0.59
2:B:33:G:N2	2:B:36:A:OP2	2.28	0.59
1:C:175:ASN:HD21	1:C:177:ASP:HB2	1.69	0.58
1:A:1212:ARG:NH2	1:A:1280:VAL:O	2.37	0.58
1:A:460:SER:OG	2:B:61:C:OP1	2.21	0.58
1:A:143:VAL:O	1:A:425:ARG:NH1	2.37	0.58
1:C:339:VAL:HG22	1:C:383:MET:HE1	1.84	0.58
1:C:1066:ASN:HD21	1:C:1069:THR:HG23	1.69	0.57
1:C:403:ARG:NH1	2:D:46:A:OP1	2.37	0.57
1:C:104:SER:OG	2:D:47:A:N3	2.37	0.57
1:A:511:HIS:HB3	1:A:593:THR:HG21	1.86	0.57
1:C:492:ILE:HG12	1:C:625:LEU:HD13	1.87	0.56
1:A:137:HIS:HA	1:A:322:ILE:HD11	1.88	0.56
1:A:665:LYS:HA	1:A:669:GLY:HA3	1.88	0.56
1:C:559:VAL:HG23	1:C:587:PHE:HB2	1.87	0.56
1:C:1099:GLU:HG2	2:D:67:C:N4	2.21	0.56
1:A:178:ASN:OD1	1:A:179:SER:OG	2.23	0.56
1:A:1277:SER:HA	1:A:1281:ILE:HG12	1.89	0.55
1:C:1162:GLU:OE1	1:C:1187:TYR:OH	2.15	0.55
1:A:369:GLN:HE21	1:A:404:THR:HG21	1.70	0.55
1:C:631:MET:O	1:C:635:ARG:HG2	2.06	0.55
1:A:107:VAL:HG13	1:A:1131:TYR:HE1	1.72	0.54
2:D:46:A:H2'	2:D:47:A:C8	2.43	0.54
1:A:269:ASP:OD1	1:A:269:ASP:N	2.40	0.54
1:A:1147:ALA:HB2	1:A:1190:VAL:HA	1.88	0.54
1:A:665:LYS:O	1:A:670:ILE:N	2.37	0.54
1:A:801:VAL:HG23	1:A:805:GLN:HG3	1.89	0.54
1:C:269:ASP:OD1	1:C:269:ASP:N	2.40	0.54
1:C:520:VAL:HG22	1:C:589:ALA:HB1	1.90	0.53
1:C:746:GLU:OE1	1:C:1353:THR:OG1	2.25	0.53
1:A:995:THR:O	1:A:998:ILE:HG22	2.09	0.53
1:A:527:VAL:HA	1:A:582:GLY:HA3	1.91	0.53
1:C:634:GLU:O	1:C:637:LYS:HG2	2.09	0.52
1:C:1210:ARG:HA	1:C:1280:VAL:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:ARG:HH12	1:C:473:ILE:HG13	1.74	0.52
1:A:447:ARG:HG3	2:B:17:A:H5'	1.91	0.52
1:A:1284:ASP:N	1:A:1284:ASP:OD1	2.42	0.52
1:A:745:ASP:OD2	1:A:938:ARG:NH1	2.41	0.52
1:C:597:LEU:O	1:C:601:ILE:HG12	2.10	0.52
1:C:423:LEU:O	1:C:427:GLU:HB2	2.10	0.52
1:A:936:ASP:OD2	1:A:940:ASN:ND2	2.44	0.51
1:C:1163:LEU:HD11	1:C:1198:LEU:HD12	1.92	0.51
1:C:1292:SER:HA	1:C:1295:ASN:HD21	1.76	0.51
1:A:241:LEU:HD11	1:A:289:LEU:HD21	1.92	0.51
1:A:373:TYR:OH	1:A:398:LEU:O	2.25	0.51
1:A:326:ASP:O	1:A:330:GLN:HG3	2.10	0.51
1:A:160:HIS:HD2	2:B:46:A:H5"	1.72	0.51
1:A:256:PHE:O	1:A:258:LEU:HD22	2.11	0.51
1:A:48:ILE:HG12	1:A:984:ALA:HB1	1.92	0.51
1:A:406:ASP:OD1	1:A:406:ASP:N	2.44	0.51
1:A:69:ARG:O	1:A:73:THR:HG23	2.10	0.51
1:C:103:GLU:HB2	1:C:106:LEU:HD12	1.93	0.51
1:C:246:LEU:HD23	1:C:300:ILE:HD13	1.93	0.51
1:A:512:SER:OG	1:A:617:GLU:OE1	2.26	0.51
1:C:212:LEU:HD21	1:C:225:LEU:HD22	1.92	0.51
1:C:386:THR:O	1:C:386:THR:OG1	2.25	0.50
1:A:1126:TRP:HB3	1:A:1131:TYR:HD2	1.75	0.50
2:B:52:A:OP2	2:B:62:G:N2	2.39	0.50
1:A:457:ARG:CZ	2:B:58:G:H5'	2.42	0.50
1:A:509:PRO:HB3	1:A:624:THR:HG21	1.92	0.50
1:A:861:ASP:O	1:A:864:ARG:HG2	2.11	0.50
1:A:898:ASP:O	1:A:905:ARG:NH2	2.45	0.50
1:C:277:ASN:OD1	1:C:278:LEU:N	2.44	0.50
1:A:143:VAL:HG21	1:A:315:ALA:HB2	1.93	0.50
1:A:1230:SER:O	1:A:1234:ASN:ND2	2.43	0.50
2:D:54:G:C6	2:D:55:C:N4	2.80	0.50
1:A:986:ASP:O	1:A:990:ASN:ND2	2.45	0.50
1:A:386:THR:O	1:A:386:THR:OG1	2.25	0.49
1:C:241:LEU:HD11	1:C:289:LEU:HD21	1.92	0.49
1:A:306:LEU:HD21	1:A:414:ILE:HD11	1.94	0.49
1:C:1254:GLN:O	1:C:1256:GLN:N	2.46	0.49
2:B:46:A:H2'	2:B:47:A:C8	2.47	0.49
1:C:184:LEU:HD12	1:C:299:ALA:HB2	1.92	0.49
1:A:246:LEU:HD23	1:A:300:ILE:HD13	1.95	0.49
1:C:116:HIS:NE2	2:D:27:G:OP1	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:O	1:A:63:ARG:N	2.46	0.49
1:A:978:ILE:HD12	1:A:1233:VAL:HG22	1.95	0.49
1:C:465:MET:HE1	1:C:482:VAL:HG13	1.94	0.49
1:A:115:ARG:HG3	2:B:26:A:H5"	1.95	0.48
1:A:810:LYS:NZ	1:A:836:TYR:O	2.38	0.48
1:A:1276:PHE:O	1:A:1280:VAL:HG22	2.12	0.48
1:C:584:GLU:O	1:C:586:ARG:N	2.44	0.48
1:A:136:TYR:CE2	1:A:402:GLN:HB3	2.49	0.48
1:A:392:LYS:C	1:A:394:ASN:H	2.17	0.48
1:A:821:ASP:HB2	1:A:828:LEU:HD21	1.95	0.48
1:C:60:GLU:O	1:C:63:ARG:N	2.47	0.48
1:C:160:HIS:CD2	2:D:46:A:H5"	2.48	0.48
1:C:71:ARG:NH1	2:D:18:C:H41	2.11	0.48
1:A:336:LYS:O	1:A:340:ARG:HG3	2.13	0.48
1:A:803:ASN:O	1:A:803:ASN:ND2	2.36	0.48
1:C:1065:THR:HG23	1:C:1071:GLU:O	2.14	0.48
1:A:226:ILE:HG21	1:A:234:LYS:HA	1.96	0.48
1:C:321:MET:HG3	1:C:402:GLN:HG3	1.94	0.47
1:C:1349:HIS:HB2	1:C:1358:THR:HB	1.96	0.47
1:C:583:VAL:HG11	1:C:587:PHE:CE2	2.50	0.47
1:C:930:HIS:O	1:C:934:ILE:HG13	2.14	0.47
1:C:847:LEU:HD23	1:C:916:PHE:HB3	1.95	0.47
1:A:256:PHE:HB2	1:A:258:LEU:HD22	1.97	0.47
1:A:478:PHE:O	1:A:482:VAL:HG22	2.15	0.47
1:A:584:GLU:O	1:A:586:ARG:N	2.48	0.47
1:C:182:ASP:OD1	1:C:183:LYS:N	2.48	0.47
1:C:841:ILE:H	1:C:854:ASN:HB3	1.80	0.47
1:A:88:ASN:OD1	1:A:89:GLU:N	2.48	0.47
1:A:979:ASN:ND2	1:A:1226:LEU:O	2.37	0.47
1:C:921:LEU:HG	1:C:1008:PHE:HE1	1.79	0.47
1:A:704:PHE:O	1:A:708:ILE:HG12	2.15	0.47
1:C:926:GLN:HG3	1:C:930:HIS:CE1	2.50	0.46
2:D:78:A:H2'	2:D:79:G:O4'	2.15	0.46
1:A:196:PHE:C	1:A:198:GLU:H	2.19	0.46
1:A:1000:LYS:HD3	1:A:1073:VAL:HG21	1.96	0.46
1:A:1099:GLU:HG2	2:B:67:C:N4	2.31	0.46
1:C:936:ASP:OD1	1:C:940:ASN:ND2	2.44	0.46
1:C:1269:ILE:HG21	1:C:1309:ILE:HD12	1.97	0.46
1:A:499:ASP:OD2	1:A:501:ASN:HB2	2.15	0.46
1:A:644:ASP:O	1:A:647:VAL:HG12	2.16	0.46
1:A:1144:LEU:O	1:A:1195:ILE:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:SER:OG	1:A:1367:GLY:HA3	2.14	0.46
1:C:758:ASN:OD1	1:C:995:THR:HG22	2.15	0.46
1:C:1045:PHE:O	1:C:1064:GLU:HG3	2.15	0.46
1:A:77:ASN:ND2	2:B:59:U:O2	2.40	0.46
1:A:427:GLU:OE2	1:A:437:ARG:NH1	2.49	0.46
1:C:609:ASN:C	1:C:611:GLU:H	2.19	0.46
1:A:478:PHE:CE2	1:A:482:VAL:HG11	2.51	0.46
1:A:760:VAL:HG11	1:A:990:ASN:O	2.16	0.46
1:A:1105:PHE:HB3	1:A:1169:MET:HE2	1.96	0.46
1:A:423:LEU:HB3	1:A:437:ARG:HG3	1.98	0.46
1:A:636:LEU:O	1:A:640:ALA:N	2.48	0.46
2:D:32:A:N6	2:D:37:U:H3	2.11	0.46
1:A:160:HIS:O	1:A:160:HIS:ND1	2.49	0.46
1:A:622:THR:HG21	1:A:635:ARG:CB	2.47	0.46
1:A:597:LEU:O	1:A:601:ILE:HG13	2.16	0.45
1:A:46:ASN:ND2	1:A:1089:MET:SD	2.89	0.45
1:A:840:ALA:O	1:A:864:ARG:NH1	2.47	0.45
1:A:891:LEU:HD12	1:A:891:LEU:HA	1.81	0.45
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.81	0.45
1:A:886:LEU:HD22	1:A:891:LEU:HD23	1.98	0.45
1:C:111:LYS:HZ1	2:D:25:U:HO2'	1.57	0.45
1:C:1146:VAL:HG21	1:C:1194:LEU:HD22	1.98	0.45
1:C:512:SER:OG	1:C:617:GLU:OE1	2.26	0.45
1:C:554:LYS:HD3	1:C:594:TYR:CZ	2.51	0.45
1:C:745:ASP:O	1:C:748:VAL:HG22	2.17	0.45
1:A:172:GLY:O	1:A:413:GLN:NE2	2.49	0.45
1:C:557:ARG:HA	1:C:595:HIS:CD2	2.52	0.45
1:A:340:ARG:NH1	2:B:40:C:H5"	2.28	0.45
1:A:913:LYS:O	1:A:917:ILE:HG12	2.17	0.45
1:A:70:ARG:NH1	2:B:61:C:OP2	2.49	0.45
1:A:1060:ARG:NH1	1:A:1064:GLU:OE2	2.44	0.45
1:A:1183:GLU:HA	1:A:1187:TYR:O	2.17	0.45
2:B:16:G:C2	2:B:17:A:C8	3.05	0.45
1:C:199:ASN:N	1:C:200:PRO:HD3	2.32	0.45
1:C:478:PHE:CE1	1:C:482:VAL:HG21	2.52	0.45
1:A:78:ARG:NH2	2:B:18:C:OP1	2.50	0.45
1:A:958:LEU:HD22	1:A:962:LEU:HD12	1.98	0.45
1:A:1146:VAL:HG22	1:A:1161:LYS:HG3	1.99	0.45
1:C:225:LEU:HD23	1:C:242:ILE:HG21	1.98	0.45
1:C:350:ILE:HD11	1:C:379:ILE:HD13	1.97	0.45
1:C:641:HIS:CE1	1:C:642:LEU:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1194:LEU:HD22	1:A:1365:LEU:HD13	1.99	0.44
1:C:324:ARG:HH21	1:C:400:ARG:NH1	2.15	0.44
1:C:596:ASP:O	1:C:600:ILE:HG12	2.16	0.44
1:A:1008:PHE:H	1:A:1008:PHE:HD2	1.65	0.44
1:A:1110:ILE:HG12	1:A:1122:ARG:NH1	2.32	0.44
1:A:1286:ASN:ND2	1:A:1332:ASP:O	2.51	0.44
1:C:1236:LEU:HD23	1:C:1236:LEU:HA	1.80	0.44
1:A:268:LYS:HA	1:A:268:LYS:HD3	1.78	0.44
1:A:477:ASN:HD22	1:A:481:VAL:HG21	1.82	0.44
1:C:850:ASP:O	1:C:851:SER:OG	2.30	0.44
1:A:784:ILE:HD11	1:A:815:TYR:HB3	2.00	0.44
1:A:820:ARG:HB2	1:A:882:TYR:OH	2.16	0.44
1:C:943:TYR:HD1	1:C:943:TYR:HA	1.63	0.44
1:A:244:LEU:HB2	1:A:250:PRO:HG3	2.00	0.44
1:A:531:THR:HG23	1:A:534:MET:H	1.83	0.44
1:C:43:ILE:HG21	1:C:45:LYS:HE2	1.98	0.44
1:C:1257:LEU:HD13	1:C:1257:LEU:HA	1.74	0.44
1:A:609:ASN:C	1:A:611:GLU:H	2.21	0.44
1:A:781:MET:HA	1:A:784:ILE:HG22	2.00	0.44
1:A:788:ILE:HG12	1:A:793:SER:HA	1.99	0.44
1:C:48:ILE:HG12	1:C:984:ALA:HB1	1.98	0.44
1:C:321:MET:HG3	1:C:402:GLN:CG	2.48	0.44
1:C:671:ARG:HB3	1:C:678:THR:HG22	2.00	0.44
1:C:58:THR:HA	1:C:731:PRO:HG2	2.00	0.43
1:A:79:ILE:HD11	1:A:163:LYS:HB2	2.00	0.43
1:A:1328:ASP:OD1	1:A:1328:ASP:N	2.49	0.43
1:C:250:PRO:HD2	1:C:264:LEU:O	2.18	0.43
1:C:363:ILE:HD13	1:C:401:LYS:HE2	2.01	0.43
1:A:452:VAL:O	1:A:465:MET:HB3	2.17	0.43
1:A:531:THR:HG21	1:A:575:PHE:CE1	2.53	0.43
1:C:106:LEU:O	1:C:111:LYS:HE3	2.18	0.43
1:A:136:TYR:HE2	1:A:402:GLN:HB3	1.82	0.43
1:A:998:ILE:HD12	1:A:998:ILE:HA	1.87	0.43
1:A:1270:ILE:HD11	1:A:1309:ILE:HG12	1.99	0.43
1:A:506:LYS:HE3	1:A:506:LYS:HB3	1.80	0.43
1:A:620:VAL:O	1:A:624:THR:OG1	2.33	0.43
1:A:763:MET:HE3	1:A:931:VAL:HG21	1.99	0.43
1:C:637:LYS:HG3	1:C:638:THR:N	2.34	0.43
1:C:99:HIS:O	1:C:103:GLU:HG2	2.19	0.43
1:A:145:SER:O	1:A:425:ARG:HD3	2.19	0.43
1:A:5:TYR:OH	1:A:754:HIS:O	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:MET:HE3	1:C:419:LEU:N	2.34	0.43
1:C:1230:SER:O	1:C:1233:VAL:HG22	2.19	0.43
1:A:189:VAL:HG12	1:A:238:PHE:CZ	2.54	0.42
1:A:847:LEU:HD13	1:A:916:PHE:HB3	2.02	0.42
1:C:163:LYS:HD3	1:C:164:PHE:CE2	2.54	0.42
1:A:1139:VAL:HA	1:A:1167:THR:HA	2.01	0.42
1:A:1142:SER:HA	1:A:1165:GLY:HA2	2.01	0.42
1:C:423:LEU:HD13	1:C:437:ARG:HG3	2.01	0.42
1:A:846:PHE:CD1	1:A:908:LEU:HD23	2.55	0.42
1:C:1144:LEU:O	1:C:1195:ILE:HA	2.19	0.42
1:A:363:ILE:HD13	1:A:401:LYS:HE2	2.00	0.42
1:A:758:ASN:HD22	1:A:954:LYS:HB2	1.84	0.42
1:A:812:TYR:CZ	1:A:816:LEU:HD11	2.55	0.42
2:B:74:A:H2'	2:B:75:A:O4'	2.20	0.42
1:C:733:ILE:HD12	1:C:733:ILE:HA	1.95	0.42
2:D:74:A:H2'	2:D:75:A:O4'	2.19	0.42
1:A:369:GLN:NE2	1:A:404:THR:HG21	2.34	0.42
1:A:678:THR:HG23	1:A:681:ASP:H	1.84	0.42
1:C:51:LEU:O	1:C:52:LEU:HD23	2.20	0.42
1:C:206:VAL:HG22	1:C:228:GLN:HB3	2.02	0.42
1:C:63:ARG:HG3	1:C:66:ARG:NH2	2.35	0.42
1:C:1243:GLU:HB2	1:C:1244:LYS:H	1.76	0.42
1:A:135:ILE:O	1:A:139:ARG:HG3	2.20	0.42
1:C:1171:ARG:O	1:C:1175:GLU:HG3	2.20	0.42
1:A:951:ARG:NH1	1:A:1010:TYR:O	2.53	0.42
1:A:1008:PHE:N	1:A:1008:PHE:CD2	2.88	0.42
1:A:186:ILE:HA	1:A:189:VAL:HG22	2.02	0.41
1:A:870:VAL:HB	1:A:871:PRO:HD2	2.02	0.41
1:C:619:ILE:HD13	1:C:651:LEU:HD21	2.02	0.41
1:A:167:HIS:HA	2:B:18:C:H4'	2.02	0.41
1:A:1006:SER:HB3	1:A:1013:TYR:HB2	2.02	0.41
1:C:645:ASP:HA	1:C:648:MET:HB3	2.02	0.41
1:A:139:ARG:O	1:A:143:VAL:HG13	2.20	0.41
1:A:184:LEU:HD22	1:A:299:ALA:HB2	2.02	0.41
1:A:1205:GLU:HB2	1:A:1348:ILE:HD11	2.01	0.41
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.89	0.41
1:A:733:ILE:HD12	1:A:733:ILE:HA	1.96	0.41
1:A:869:ASN:HD21	1:A:908:LEU:HB2	1.86	0.41
1:C:419:LEU:HD21	1:C:440:ILE:HG22	2.03	0.41
1:C:503:PRO:HG2	1:C:714:SER:HB2	2.03	0.41
1:A:563:GLN:O	1:A:567:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:TYR:CE1	1:C:756:PRO:HB3	2.55	0.41
1:C:305:ILE:HG22	1:C:306:LEU:H	1.85	0.41
1:C:654:ARG:HA	1:C:654:ARG:HD2	1.93	0.41
1:A:185:PHE:O	1:A:189:VAL:HG13	2.20	0.41
1:A:258:LEU:HD11	1:A:281:GLN:HB3	2.01	0.41
1:C:686:ASP:OD2	1:C:690:ASN:HA	2.21	0.41
1:C:1110:ILE:HG23	1:C:1122:ARG:HD2	2.01	0.41
1:A:469:SER:OG	1:A:470:GLU:N	2.54	0.41
1:A:527:VAL:HG22	1:A:583:VAL:HG23	2.03	0.41
1:A:812:TYR:O	1:A:816:LEU:HG	2.21	0.41
1:C:548:ILE:O	1:C:552:LEU:HB2	2.21	0.41
1:C:590:SER:O	1:C:591:LEU:HB2	2.21	0.41
1:C:666:LEU:O	1:C:679:ILE:HD13	2.20	0.41
1:C:133:PRO:HG2	1:C:137:HIS:CE1	2.56	0.41
1:C:974:LYS:HE2	1:C:982:HIS:HB2	2.02	0.41
1:A:49:GLY:HA2	1:A:1092:VAL:HG12	2.03	0.40
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.95	0.40
1:A:1305:GLN:O	1:A:1309:ILE:HG13	2.21	0.40
1:C:457:ARG:NH2	2:D:57:A:OP1	2.44	0.40
1:C:630:GLU:O	1:C:633:GLU:HG2	2.21	0.40
1:C:995:THR:O	1:C:998:ILE:HG22	2.21	0.40
1:A:394:ASN:C	1:A:396:GLU:H	2.24	0.40
1:C:135:ILE:HG21	1:C:160:HIS:CE1	2.56	0.40
1:A:163:LYS:HD3	1:A:164:PHE:CZ	2.56	0.40
1:A:962:LEU:HD23	1:A:962:LEU:HA	1.87	0.40
1:A:1008:PHE:HD2	1:A:1008:PHE:N	2.19	0.40
1:C:404:THR:HB	1:C:405:PHE:H	1.75	0.40
1:C:1144:LEU:HB3	1:C:1196:ILE:HB	2.03	0.40
1:C:1226:LEU:HD13	1:C:1276:PHE:CG	2.56	0.40
1:C:502:LEU:HD23	1:C:505:GLU:HG3	2.02	0.40
1:C:700:ASP:OD2	1:C:701:SER:N	2.53	0.40
1:C:1215:ALA:HB2	1:C:1221:GLN:HG3	2.03	0.40
1:A:18:TRP:CE3	1:A:747:LEU:HD11	2.57	0.40
1:A:185:PHE:CE1	1:A:225:LEU:HD21	2.56	0.40
1:A:621:LEU:O	1:A:625:LEU:HD13	2.22	0.40
1:A:763:MET:CE	1:A:931:VAL:HG21	2.52	0.40
1:C:488:ALA:O	1:C:492:ILE:HG13	2.22	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	1325/1369 (97%)	1240 (94%)	81 (6%)	4 (0%)	41	73
1	C	1138/1369 (83%)	1075 (94%)	59 (5%)	4 (0%)	34	69
All	All	2463/2738 (90%)	2315 (94%)	140 (6%)	8 (0%)	41	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ASP
1	C	257	ASP
1	C	1255	LYS
1	C	1259	VAL
1	A	688	PHE
1	C	1254	GLN
1	A	946	ASN
1	A	1018	VAL

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	1026/1226 (84%)	985 (96%)	41 (4%)	31	65
1	C	920/1226 (75%)	903 (98%)	17 (2%)	59	82
All	All	1946/2452 (79%)	1888 (97%)	58 (3%)	41	71

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	SER
1	A	80	CYS
1	A	102	GLU
1	A	121	ASN
1	A	386	THR
1	A	406	ASP
1	A	419	LEU
1	A	425	ARG
1	A	428	ASP
1	A	479	GLU
1	A	502	LEU
1	A	506	LYS
1	A	525	THR
1	A	567	ASP
1	A	578	VAL
1	A	597	LEU
1	A	607	LEU
1	A	614	ASP
1	A	624	THR
1	A	627	GLU
1	A	686	ASP
1	A	709	GLN
1	A	718	ASP
1	A	779	GLU
1	A	784	ILE
1	A	790	GLU
1	A	803	ASN
1	A	804	THR
1	A	837	ASP
1	A	891	LEU
1	A	908	LEU
1	A	947	ASP
1	A	1007	GLU
1	A	1008	PHE
1	A	1037	PHE
1	A	1143	VAL
1	A	1179	ILE
1	A	1242	TYR
1	A	1267	ASP
1	A	1284	ASP
1	A	1368	ASP
1	C	104	SER
1	C	324	ARG

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Mol	Chain	Res	Type
1	C	419	LEU
1	C	476	TRP
1	C	480	GLU
1	C	610	GLU
1	C	642	LEU
1	C	690	ASN
1	C	723	HIS
1	C	847	LEU
1	C	908	LEU
1	C	943	TYR
1	C	1008	PHE
1	C	1190	VAL
1	C	1233	VAL
1	C	1241	HIS
1	C	1243	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	GLN
1	C	1295	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	71/85 (83%)	18 (25%)	1 (1%)
2	D	71/85 (83%)	16 (22%)	1 (1%)
All	All	142/170 (83%)	34 (23%)	2 (1%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	A
2	B	24	U
2	B	28	A
2	B	29	G
2	B	31	U
2	B	32	A
2	B	37	U
2	B	38	A

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Mol	Chain	Res	Type
2	B	40	C
2	B	43	G
2	B	51	A
2	B	56	U
2	B	59	U
2	B	63	U
2	B	68	A
2	B	73	G
2	B	77	A
2	B	79	G
2	D	12	A
2	D	24	U
2	D	28	A
2	D	29	G
2	D	31	U
2	D	32	A
2	D	37	U
2	D	40	C
2	D	51	A
2	D	56	U
2	D	59	U
2	D	63	U
2	D	68	A
2	D	73	G
2	D	77	A
2	D	79	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	42	A
2	D	78	A

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	1335/1369 (97%)	-0.04	37 (2%) 53 30	29, 86, 134, 177	0
1	C	1160/1369 (84%)	-0.25	6 (0%) 91 81	29, 61, 116, 150	0
2	B	72/85 (84%)	-0.22	0 100 100	34, 70, 202, 227	0
2	D	72/85 (84%)	-0.28	0 100 100	30, 48, 138, 182	0
All	All	2639/2908 (90%)	-0.14	43 (1%) 72 51	29, 72, 128, 227	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	ILE	5.4
1	A	378	PRO	5.1
1	A	335	LEU	4.8
1	A	1247	GLY	4.7
1	A	517	TYR	3.5
1	A	376	ILE	3.4
1	A	331	ASP	3.4
1	A	904	GLU	3.4
1	A	689	ALA	3.4
1	A	581	SER	3.3
1	A	580	ILE	3.2
1	A	332	LEU	3.2
1	A	140	LYS	3.1
1	A	384	ASP	3.0
1	A	328	HIS	2.9
1	A	538	ALA	2.9
1	C	581	SER	2.9
1	A	381	GLU	2.7
1	A	383	MET	2.7
1	A	1054	ASN	2.7
1	A	144	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	872	SER	2.6
1	A	156	LEU	2.6
1	A	811	LEU	2.6
1	C	996	ALA	2.4
1	A	823	TYR	2.4
1	A	136	TYR	2.4
1	A	433	LEU	2.4
1	A	1246	LYS	2.3
1	A	1050	ILE	2.3
1	A	582	GLY	2.3
1	C	1070	GLY	2.3
1	C	587	PHE	2.3
1	A	693	PHE	2.2
1	A	861	ASP	2.2
1	A	402	GLN	2.2
1	C	590	SER	2.2
1	A	440	ILE	2.1
1	A	908	LEU	2.1
1	C	851	SER	2.1
1	A	197	GLU	2.1
1	A	810	LYS	2.1
1	A	1248	SER	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.