



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:34 AM UTC

PDB ID : 4ZT9 / pdb_00004zt9
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

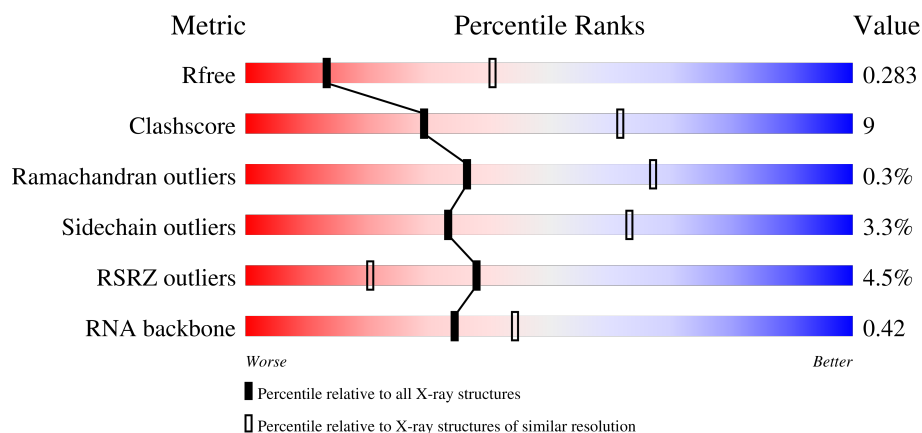
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	1369	 6% 75% 22% ..
1	C	1369	 3% 67% 17% • 15%
2	B	85	 % 41% 38% 6% 15%
2	D	85	 46% 32% 7% 15%

2 Entry composition

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
1	A	1335	Total	C	N	O	S	0	0	0
			10208	6499	1738	1952	19			
1	C	1160	Total	C	N	O	S	0	0	0
			8980	5725	1550	1689	16			

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

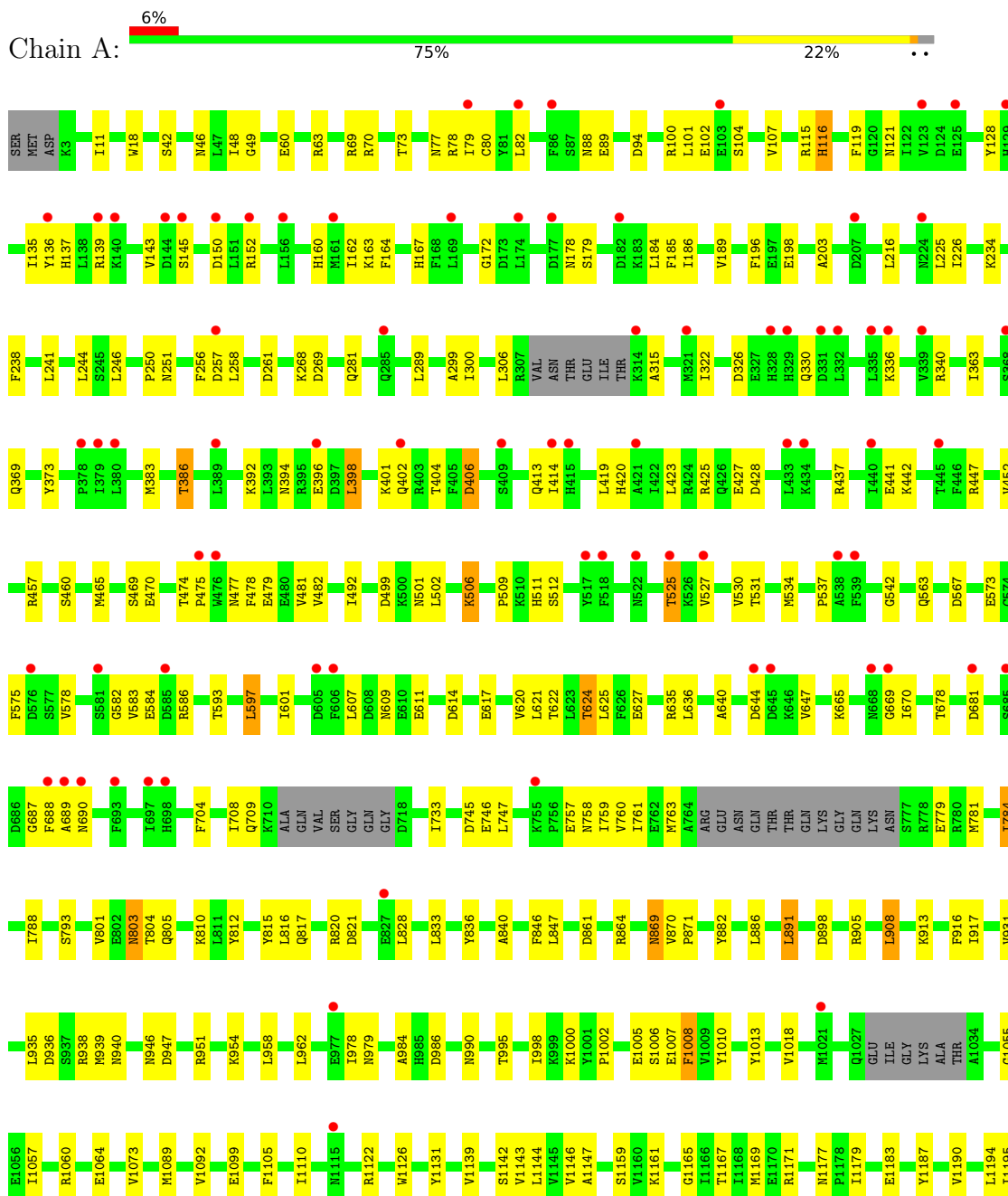
- Molecule 2 is a RNA chain called single-guide RNA.

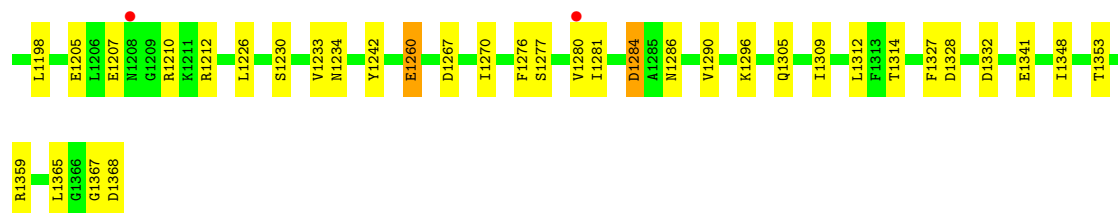
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	72	Total	C	N	O	P	0	0	0
			1545	692	285	496	72			
2	D	72	Total	C	N	O	P	0	0	0
			1545	692	285	496	72			

3 Residue-property plots

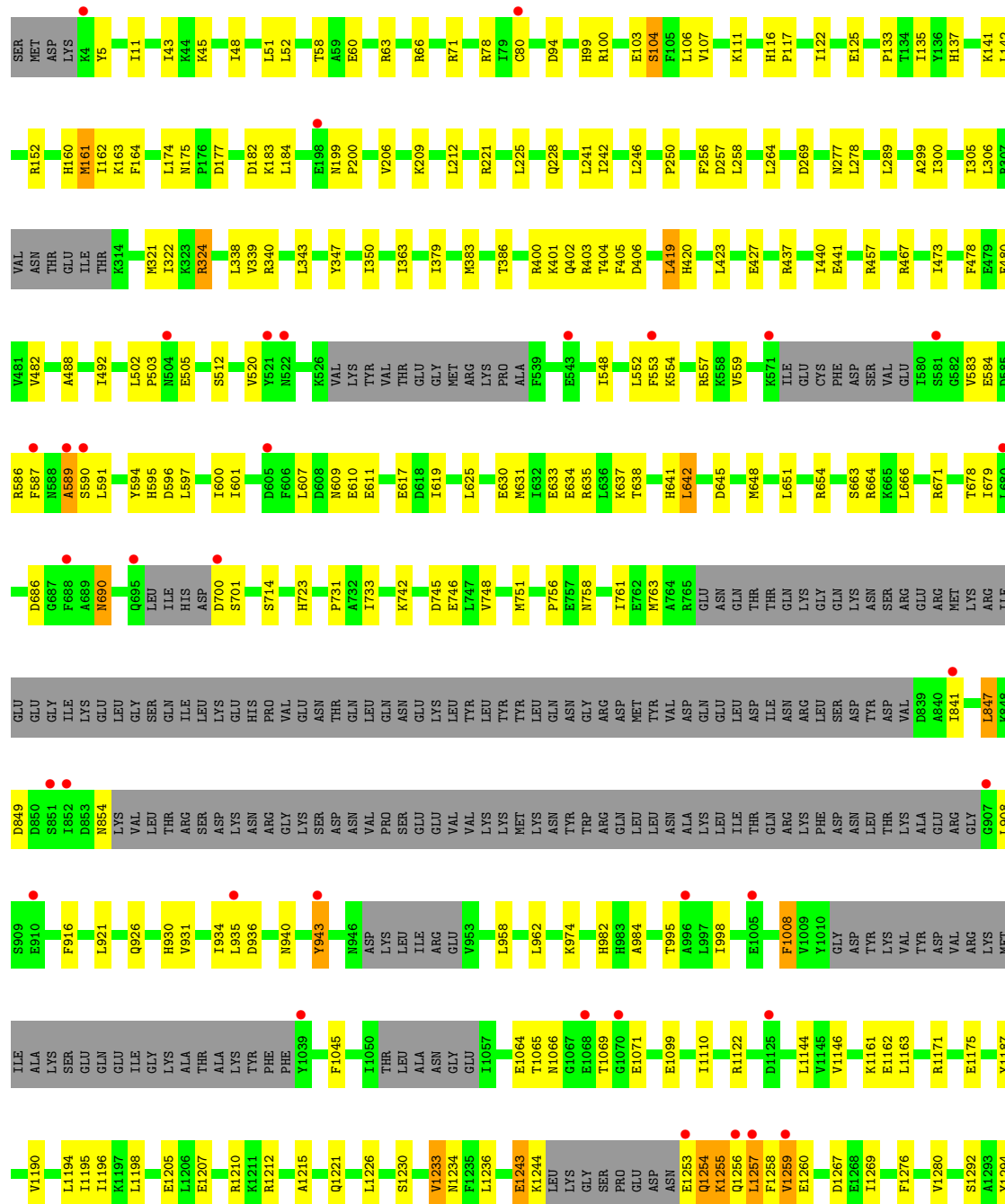
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

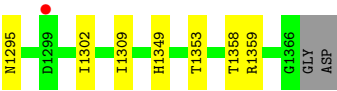
• Molecule 1: CRISPR-associated endonuclease Cas9



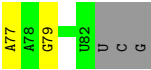
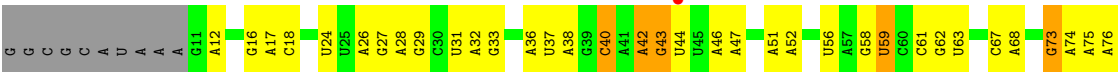


● Molecule 1: CRISPR-associated endonuclease Cas9

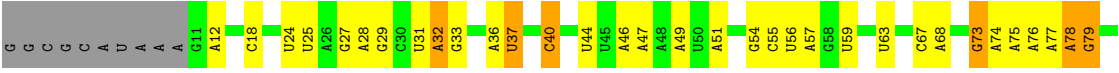




● Molecule 2: single-guide RNA



● Molecule 2: single-guide RNA



4 Data and refinement statistics

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 49.36 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.36-3.10) 96.2 (49.36-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.243 , 0.284 0.246 , 0.283	Depositor DCC
R_{free} test set	3873 reflections (4.85%)	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)	0.27 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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.*

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	0.48	0/10393	0.76	10/14104 (0.1%)
1	C	0.57	2/9136 (0.0%)	0.79	2/12364 (0.0%)
2	B	0.38	0/1732	0.44	0/2698
2	D	0.48	0/1732	0.46	0/2698
All	All	0.52	2/22993 (0.0%)	0.73	12/31864 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	80	CYS	CB-SG	-11.93	1.41	1.81
1	C	161	MET	C-O	-5.58	1.17	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	HIS	CA-C-N	6.05	125.26	118.97
1	A	116	HIS	C-N-CA	6.05	125.26	118.97
1	A	1171	ARG	N-CA-C	5.81	117.28	111.07
1	C	589	ALA	N-CA-C	5.47	118.17	111.82
1	A	1198	LEU	CA-C-N	5.33	125.33	120.21
1	A	1198	LEU	C-N-CA	5.33	125.33	120.21
1	A	1327	PHE	CB-CA-C	-5.18	110.18	117.23
1	A	1177	ASN	CA-C-N	5.17	124.49	118.85
1	A	1177	ASN	C-N-CA	5.17	124.49	118.85
1	C	347	TYR	N-CA-C	-5.17	106.66	113.12
1	A	1055	GLY	N-CA-C	-5.11	107.48	114.64
1	A	542	GLY	N-CA-C	5.08	118.82	112.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10208	0	9648	186	0
1	C	8980	0	8681	162	0
2	B	1545	0	774	23	0
2	D	1545	0	774	19	0
All	All	22278	0	19877	363	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 9.

All (363) 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	1.12
1:C:161:MET:HE3	1:C:419:LEU:HB2	1.32	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	1.95	0.97
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	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:339:VAL:HG22	1:C:383:MET:HE1	1.74	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:C:763:MET:HE1	1:C:931:VAL:HG21	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:343:LEU:HD13	1:C:383:MET:HE2	1.83	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
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	2.32	0.60
1:C:161:MET:HE3	1:C:419:LEU:CA	2.27	0.60
1:A:492:ILE:HG12	1:A:625:LEU:HD23	1.82	0.60
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: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:101:LEU:O	1:A:104:SER:OG	2.14	0.56
1:A:763:MET:HE1	1:A:931:VAL:HG21	1.86	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:386:THR:O	1:A:386:THR:OG1	2.25	0.55
1:A:107:VAL:HG13	1:A:1131:TYR:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:392:LYS:C	1:A:394:ASN:H	2.17	0.52
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
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:A:196:PHE:C	1:A:198:GLU:H	2.19	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:609:ASN:C	1:C:611:GLU:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:60:GLU:O	1:A:63:ARG:N	2.46	0.49
1:A:609:ASN:C	1:A:611:GLU:H	2.21	0.49
1:A:978:ILE:HD12	1:A:1233:VAL:HG22	1.95	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:11:ILE:HD12	1:A:763:MET:HE2	1.93	0.48
1:A:1105:PHE:HB3	1:A:1169:MET:HE2	1.96	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:821:ASP:HB2	1:A:828:LEU:HD21	1.95	0.48
1:C:11:ILE:HD12	1:C:763:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:1146:VAL:HG21	1:C:1194:LEU:HD22	1.98	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:A:394:ASN:C	1:A:396:GLU:H	2.24	0.45
1:C:111:LYS:HZ1	2:D:25:U:HO2'	1.59	0.45
1:C:557:ARG:HA	1:C:595:HIS:CD2	2.52	0.45
1:C:751:MET:HE3	1:C:751:MET:HB3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:512:SER:OG	1:C:617:GLU:OE1	2.26	0.43
1:C:648:MET:HE2	1:C:648:MET:HB2	1.87	0.43
1:A:1000:LYS:C	1:A:1002:PRO:HD3	2.44	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:C:1253:GLU:C	1:C:1255:LYS:H	2.22	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:573:GLU:C	1:A:575:PHE:H	2.28	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:A:759:ILE:HD11	1:A:939:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:637:LYS:HG3	1:C:638:THR:N	2.34	0.41
1:C:161:MET:HE3	1:C:419:LEU:N	2.36	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
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:C:135:ILE:HG21	1:C:160:HIS:CE1	2.56	0.40
1:C:1207:GLU:CD	1:C:1210:ARG:HH21	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	67
1	C	1138/1369 (83%)	1075 (94%)	59 (5%)	4 (0%)	30	61
All	All	2463/2738 (90%)	2315 (94%)	140 (6%)	8 (0%)	36	67

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

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Mol	Chain	Res	Type
1	A	946	ASN
1	A	1018	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	1026/1226 (84%)	985 (96%)	41 (4%)	28	60
1	C	920/1226 (75%)	896 (97%)	24 (3%)	40	68
All	All	1946/2452 (79%)	1881 (97%)	65 (3%)	33	63

All (65) 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	383	MET
1	A	386	THR
1	A	398	LEU
1	A	406	ASP
1	A	419	LEU
1	A	428	ASP
1	A	479	GLU
1	A	502	LEU
1	A	506	LYS
1	A	525	THR
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	709	GLN

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Mol	Chain	Res	Type
1	A	757	GLU
1	A	779	GLU
1	A	784	ILE
1	A	803	ASN
1	A	804	THR
1	A	869	ASN
1	A	891	LEU
1	A	908	LEU
1	A	947	ASP
1	A	1007	GLU
1	A	1008	PHE
1	A	1057	ILE
1	A	1143	VAL
1	A	1179	ILE
1	A	1260	GLU
1	A	1267	ASP
1	A	1284	ASP
1	A	1296	LYS
1	A	1314	THR
1	A	1368	ASP
1	C	104	SER
1	C	107	VAL
1	C	122	ILE
1	C	141	LYS
1	C	174	LEU
1	C	324	ARG
1	C	419	LEU
1	C	480	GLU
1	C	607	LEU
1	C	610	GLU
1	C	642	LEU
1	C	690	ASN
1	C	723	HIS
1	C	742	LYS
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	1243	GLU
1	C	1257	LEU

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Mol	Chain	Res	Type
1	C	1259	VAL
1	C	1302	ILE

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	41	HIS
1	A	121	ASN
1	A	369	GLN
1	A	459	ASN
1	A	1101	GLN
1	A	1350	GLN
1	C	41	HIS
1	C	46	ASN
1	C	459	ASN
1	C	511	HIS
1	C	739	GLN
1	C	1295	ASN

5.3.3 RNA ⓘ

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
2	B	40	C
2	B	43	G
2	B	51	A

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Mol	Chain	Res	Type
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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(Å ²)	Q<0.9
1	A	1335/1369 (97%)	0.50	81 (6%) 27 15	29, 86, 134, 177	0
1	C	1160/1369 (84%)	0.18	36 (3%) 51 30	29, 61, 116, 150	0
2	B	72/85 (84%)	0.06	1 (1%) 73 53	34, 70, 202, 227	0
2	D	72/85 (84%)	-0.45	0 100 100	30, 48, 138, 182	0
All	All	2639/2908 (90%)	0.32	118 (4%) 38 20	29, 72, 128, 227	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	ASP	4.7
1	A	335	LEU	4.7
1	A	693	PHE	4.1
1	A	396	GLU	4.0
1	A	332	LEU	4.0
1	A	144	ASP	4.0
1	A	517	TYR	4.0
1	A	182	ASP	3.9
1	A	328	HIS	3.9
1	A	440	ILE	3.8
1	A	688	PHE	3.7
1	A	136	TYR	3.6
1	A	689	ALA	3.6
1	C	522	ASN	3.6
1	A	140	LYS	3.5
1	A	150	ASP	3.4
1	A	79	ILE	3.3
1	C	688	PHE	3.3
1	A	606	PHE	3.2
1	A	685	SER	3.2
1	A	152	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	590	SER	3.1
1	C	1299	ASP	3.1
1	A	86	PHE	3.1
1	C	198	GLU	3.1
1	A	156	LEU	3.0
1	A	285	GLN	3.0
1	A	525	THR	3.0
1	C	605	ASP	3.0
1	A	827	GLU	2.9
1	A	161	MET	2.9
1	C	851	SER	2.9
1	C	1005	GLU	2.8
1	A	379	ILE	2.8
1	A	389	LEU	2.8
1	A	414	ILE	2.8
1	A	103	GLU	2.8
1	A	378	PRO	2.8
1	C	852	ILE	2.8
1	A	690	ASN	2.7
1	A	538	ALA	2.7
1	C	1259	VAL	2.7
1	A	669	GLY	2.7
1	C	1068	GLU	2.7
1	A	476	TRP	2.7
1	A	475	PRO	2.6
1	A	421	ALA	2.6
1	A	977	GLU	2.6
1	C	680	LEU	2.6
1	A	1115	ASN	2.6
1	C	1253	GLU	2.6
1	C	943	TYR	2.5
1	A	409	SER	2.5
1	C	935	LEU	2.5
1	A	434	LYS	2.5
1	A	336	LYS	2.5
1	C	1257	LEU	2.5
1	C	4	LYS	2.5
1	C	521	TYR	2.5
1	C	907	GLY	2.5
1	A	605	ASP	2.4
1	C	1256	GLN	2.4
1	C	910	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	668	ASN	2.4
1	A	224	ASN	2.4
1	C	581	SER	2.4
1	C	1070	GLY	2.4
1	A	518	PHE	2.4
1	A	339	VAL	2.4
1	C	1039	TYR	2.3
1	C	543	GLU	2.3
1	A	129	HIS	2.3
1	C	589	ALA	2.3
1	A	585	ASP	2.3
1	A	402	GLN	2.3
1	A	125	GLU	2.3
1	A	123	VAL	2.3
1	A	169	LEU	2.3
1	A	207	ASP	2.3
1	C	700	ASP	2.3
1	C	996	ALA	2.3
1	C	571	LYS	2.3
1	A	681	ASP	2.2
1	A	380	LEU	2.2
1	C	553	PHE	2.2
1	A	329	HIS	2.2
1	A	527	VAL	2.2
1	A	539	PHE	2.2
1	A	445	THR	2.2
1	A	314	LYS	2.2
1	A	576	ASP	2.2
1	A	174	LEU	2.2
1	A	257	ASP	2.2
1	C	841	ILE	2.1
1	A	368	SER	2.1
1	A	139	ARG	2.1
1	C	504	ASN	2.1
1	A	645	ASP	2.1
1	C	1125	ASP	2.1
1	A	415	HIS	2.1
1	A	321	MET	2.1
1	A	581	SER	2.1
1	A	1208	ASN	2.1
1	C	80	CYS	2.1
1	A	755	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	145	SER	2.1
1	C	587	PHE	2.1
1	A	82	LEU	2.1
1	A	697	ILE	2.1
1	A	644	ASP	2.1
1	C	695	GLN	2.1
1	A	1280	VAL	2.0
2	B	44	U	2.0
1	A	1021	MET	2.0
1	A	177	ASP	2.0
1	A	433	LEU	2.0
1	A	522	ASN	2.0
1	A	698	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.