



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2016 – 12:32 AM EDT

PDB ID : 5F9R
Title : Crystal structure of catalytically-active Streptococcus pyogenes CRISPR-Cas9 in complex with single-guided RNA and double-stranded DNA primed for target DNA cleavage
Authors : Jiang, F.; Doudna, J.A.
Deposited on : 2015-12-10
Resolution : 3.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

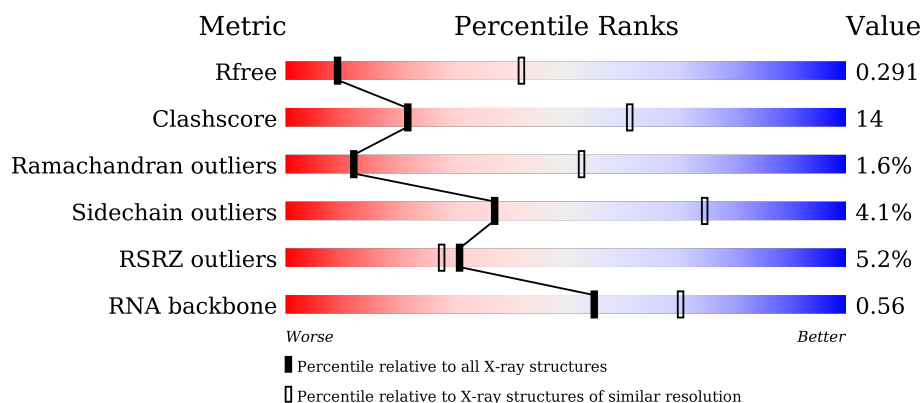
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	B	1368	<div> <div>5%</div> <div>68%</div> <div>29%</div> <div>.</div> </div>
2	A	118	<div> <div>9%</div> <div>37%</div> <div>43%</div> <div>14%</div> <div>..</div> </div>
3	C	30	<div> <div>40%</div> <div>57%</div> <div>.</div> </div>
4	D	30	<div> <div>17%</div> <div>30%</div> <div>17%</div> <div>37%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13652 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/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1362	Total	C	N	O	S	0	0	0
			10146	6419	1727	1978	22			

- Molecule 2 is a RNA chain called RNA (116-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	116	Total	C	N	O	P	0	0	0
			2494	1112	455	809	118			

- Molecule 3 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	30	Total	C	N	O	P	0	0	0
			601	289	101	182	29			

- Molecule 4 is a DNA chain called DNA (5'-D(P*AP*TP*GP*AP*GP*AP*CP*GP*CP*TP*GP*GP*AP*GP*TP*AP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	19	Total	C	N	O	P	0	0	0
			396	187	77	113	19			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

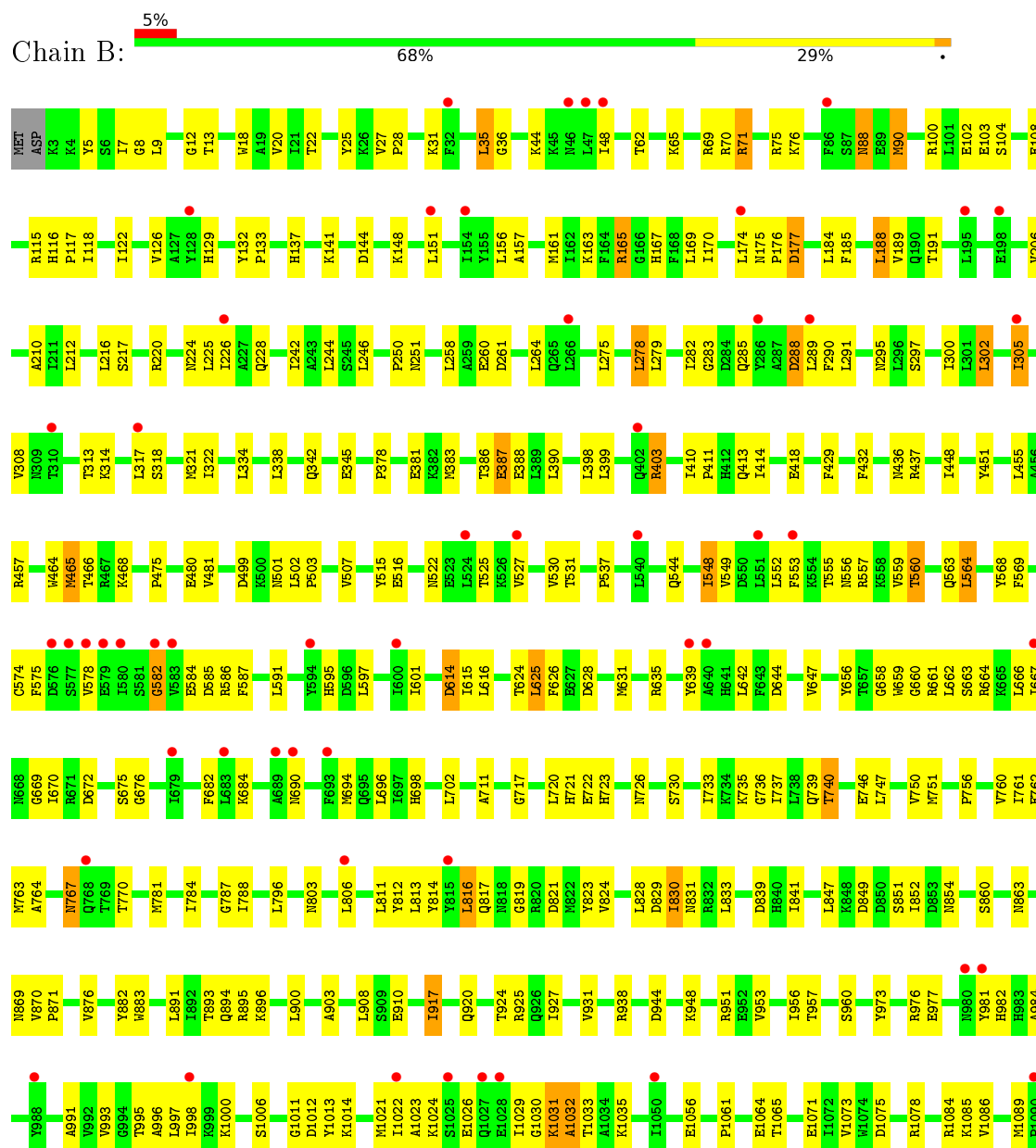


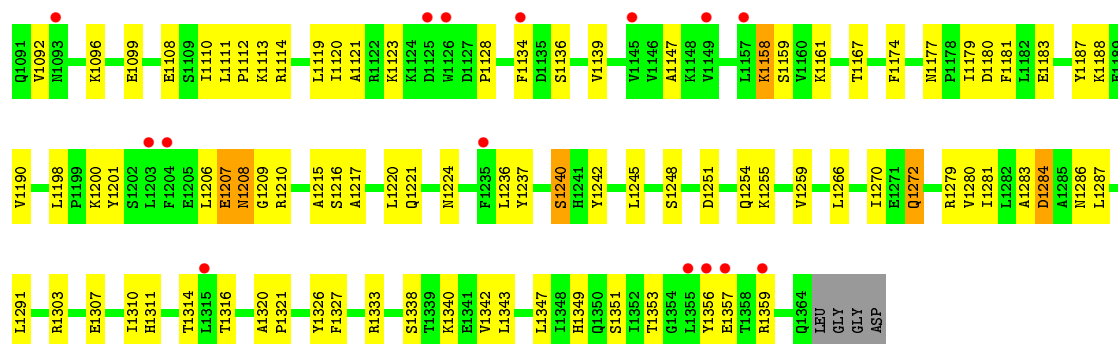
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

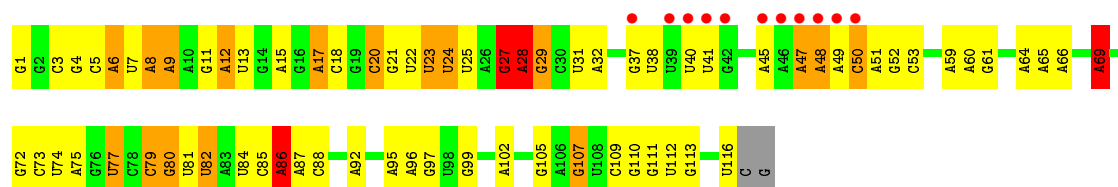
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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/Csn1

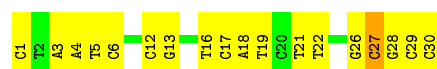




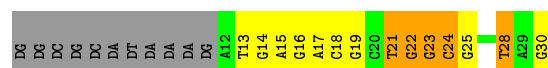
• Molecule 2: RNA (116-MER)



• Molecule 3: DNA (30-MER)



• Molecule 4: DNA (5'-D(P*AP*TP*GP*AP*GP*AP*CP*GP*CP*TP*GP*GP*AP*GP*TP*A P*CP*AP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	147.94Å 230.10Å 417.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.72 – 3.40 69.72 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (69.72-3.40) 98.8 (69.72-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.237 , 0.299 0.238 , 0.291	Depositor DCC
R_{free} test set	4575 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	112.3	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 89.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 48413 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13652	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GTP, SO4

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	B	0.49	0/10323	0.73	2/14064 (0.0%)
2	A	0.71	1/2758 (0.0%)	1.33	31/4297 (0.7%)
3	C	1.27	2/670 (0.3%)	1.27	5/1030 (0.5%)
4	D	1.18	1/445 (0.2%)	1.16	5/686 (0.7%)
All	All	0.63	4/14196 (0.0%)	0.94	43/20077 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	19	DT	C3'-O3'	-8.54	1.32	1.44
4	D	23	DG	C3'-O3'	-5.72	1.36	1.44
3	C	22	DT	C3'-O3'	-5.56	1.36	1.44
2	A	13	U	N1-C6	-5.14	1.33	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	8	A	N9-C1'-C2'	-8.40	102.76	112.00
2	A	12	A	C8-N9-C4	8.27	109.11	105.80
2	A	12	A	C2-N3-C4	-7.65	106.77	110.60
2	A	69	A	N1-C6-N6	7.08	122.85	118.60
2	A	82	U	C5-C6-N1	7.03	126.22	122.70
2	A	13	U	C5-C6-N1	-6.92	119.24	122.70
2	A	79	C	N1-C2-O2	-6.80	114.82	118.90
2	A	13	U	OP1-P-OP2	6.54	129.42	119.60
2	A	6	A	O5'-P-OP1	-6.49	99.86	105.70
2	A	69	A	C6-C5-N7	-6.17	127.98	132.30
2	A	69	A	N7-C8-N9	6.08	116.84	113.80
2	A	9	A	N1-C6-N6	-6.06	114.96	118.60
3	C	27	DC	O4'-C4'-C3'	-5.92	102.13	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	69	A	C5-N7-C8	-5.92	100.94	103.90
2	A	27	G	N9-C1'-C2'	-5.92	105.49	112.00
2	A	13	U	C6-N1-C2	5.78	124.47	121.00
2	A	12	A	N9-C4-C5	-5.74	103.51	105.80
2	A	21	G	O5'-P-OP1	5.72	117.56	110.70
4	D	24	DC	C1'-O4'-C4'	-5.68	104.42	110.10
3	C	21	DT	N3-C4-O4	5.66	123.30	119.90
2	A	66	A	O5'-P-OP2	5.63	117.45	110.70
2	A	82	U	N3-C4-O4	5.61	123.32	119.40
2	A	47	A	OP1-P-O3'	5.60	117.51	105.20
4	D	28	DT	C1'-O4'-C4'	-5.58	104.52	110.10
3	C	22	DT	O5'-P-OP2	-5.49	100.76	105.70
2	A	9	A	N7-C8-N9	-5.38	111.11	113.80
2	A	23	U	C6-N1-C2	5.36	124.22	121.00
2	A	7	U	C2-N1-C1'	-5.35	111.28	117.70
1	B	616	LEU	CA-CB-CG	5.34	127.59	115.30
4	D	22	DG	O4'-C4'-C3'	-5.34	102.36	104.50
2	A	80	G	C2-N3-C4	-5.34	109.23	111.90
4	D	22	DG	C1'-O4'-C4'	-5.29	104.81	110.10
2	A	69	A	C5-C6-N6	-5.27	119.49	123.70
2	A	86	A	O4'-C1'-N9	-5.24	104.01	108.20
2	A	79	C	N3-C2-O2	5.21	125.55	121.90
3	C	21	DT	O5'-P-OP1	-5.16	101.05	105.70
2	A	7	U	C5-C6-N1	-5.14	120.13	122.70
3	C	21	DT	C5-C4-O4	-5.12	121.32	124.90
1	B	35	LEU	CA-CB-CG	5.11	127.06	115.30
2	A	28	A	O4'-C1'-N9	-5.06	104.15	108.20
4	D	21	DT	O5'-P-OP2	5.02	116.73	110.70
2	A	23	U	O5'-P-OP1	5.01	116.72	110.70
2	A	9	A	C6-C5-N7	5.01	135.81	132.30

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	B	10146	0	9339	290	0
2	A	2494	0	1248	57	0
3	C	601	0	341	15	0
4	D	396	0	214	15	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
All	All	13652	0	11142	346	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 14.

All (346) 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:B:957:THR:OG1	2:A:1:GTP:O2A	1.94	0.86
1:B:841:ILE:HD12	1:B:900:LEU:HD21	1.63	0.80
1:B:1236:LEU:O	1:B:1240:SER:OG	2.00	0.80
1:B:1065:THR:OG1	1:B:1071:GLU:O	1.99	0.79
4:D:16:DG:N7	4:D:17:DA:N6	2.31	0.79
1:B:1272:GLN:NE2	2:A:107:G:O6	2.16	0.79
3:C:1:DC:O2	4:D:30:DG:N2	2.12	0.78
1:B:730:SER:HB3	2:A:12:A:O3'	1.82	0.78
2:A:37:G:O6	2:A:50:C:N4	2.17	0.77
1:B:1031:LYS:O	1:B:1035:LYS:N	2.18	0.76
1:B:386:THR:OG1	1:B:387:GLU:N	2.18	0.76
1:B:1215:ALA:HB2	1:B:1221:GLN:HG3	1.67	0.75
1:B:1357:GLU:OE1	1:B:1359:ARG:NH1	2.20	0.75
1:B:770:THR:HG22	1:B:1032:ALA:HB3	1.71	0.72
1:B:1120:ILE:HB	1:B:1134:PHE:HB2	1.71	0.72
1:B:720:LEU:HD12	1:B:938:ARG:HH21	1.55	0.71
1:B:781:MET:HG2	1:B:803:ASN:HB3	1.71	0.70
1:B:893:THR:HG23	1:B:896:LYS:H	1.57	0.69
1:B:69:ARG:HH12	2:A:80:G:H3'	1.58	0.69
1:B:1356:TYR:HB3	2:A:99:G:C6	2.28	0.68
1:B:465:MET:HG2	1:B:466:THR:N	2.06	0.68
1:B:803:ASN:HA	1:B:806:LEU:HB3	1.75	0.68
1:B:721:HIS:O	1:B:723:HIS:N	2.26	0.68
1:B:951:ARG:HH12	1:B:1012:ASP:H	1.42	0.68
2:A:3:C:H2'	2:A:4:G:C8	2.29	0.67
1:B:1251:ASP:HA	1:B:1254:GLN:HG3	1.76	0.67
1:B:1030:GLY:O	1:B:1032:ALA:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LEU:HD22	1:B:305:ILE:HB	1.77	0.67
1:B:432:PHE:O	1:B:436:ASN:ND2	2.28	0.67
1:B:410:ILE:HG23	1:B:414:ILE:HD11	1.77	0.66
4:D:21:DT:H2''	4:D:22:DG:C8	2.30	0.66
1:B:1000:LYS:HA	1:B:1073:VAL:HG11	1.77	0.66
1:B:869:ASN:OD1	1:B:870:VAL:N	2.29	0.65
1:B:552:LEU:HB3	1:B:559:VAL:HG21	1.77	0.65
1:B:398:LEU:HD13	1:B:399:LEU:HD13	1.78	0.64
1:B:1119:LEU:HB3	1:B:1128:PRO:HB2	1.79	0.64
1:B:1021:MET:HG3	1:B:1022:ILE:HG23	1.80	0.64
1:B:1338:SER:HB3	1:B:1340:LYS:HD3	1.80	0.63
2:A:4:G:H2'	2:A:5:C:C6	2.34	0.63
1:B:1147:ALA:HB1	1:B:1188:LYS:O	1.98	0.63
1:B:264:LEU:HD11	1:B:278:LEU:HD22	1.80	0.62
1:B:457:ARG:HH21	2:A:75:A:H5''	1.64	0.62
4:D:17:DA:H5'	4:D:17:DA:C8	2.35	0.62
2:A:5:C:H2'	2:A:6:A:C8	2.35	0.61
1:B:951:ARG:NH1	1:B:1012:ASP:H	1.98	0.61
2:A:51:A:H2'	2:A:52:G:C8	2.36	0.61
1:B:62:THR:HG23	2:A:81:U:H2'	1.82	0.61
2:A:51:A:H2'	2:A:52:G:H8	1.65	0.61
1:B:750:VAL:HG22	1:B:1356:TYR:OH	2.01	0.61
1:B:398:LEU:CD1	1:B:399:LEU:HD13	2.31	0.60
1:B:910:GLU:HB2	1:B:1311:HIS:NE2	2.15	0.60
1:B:760:VAL:HG22	1:B:956:ILE:HD12	1.82	0.60
2:A:3:C:H2'	2:A:4:G:H8	1.65	0.60
1:B:5:TYR:CE1	1:B:756:PRO:HB3	2.36	0.60
4:D:24:DC:H2''	4:D:25:DG:C8	2.36	0.60
1:B:12:GLY:HA2	1:B:924:THR:HG22	1.83	0.60
1:B:817:GLN:O	1:B:882:TYR:OH	2.19	0.59
1:B:9:LEU:HB2	1:B:761:ILE:HG22	1.85	0.59
1:B:1099:GLU:HB2	2:A:85:C:H42	1.68	0.59
1:B:552:LEU:HD13	1:B:559:VAL:HG11	1.85	0.59
1:B:1206:LEU:HD22	1:B:1210:ARG:HH12	1.66	0.59
1:B:1207:GLU:O	1:B:1209:GLY:N	2.36	0.59
1:B:1174:PHE:HD1	1:B:1181:PHE:CD1	2.20	0.58
1:B:951:ARG:HH22	1:B:1011:GLY:HA3	1.67	0.58
1:B:883:TRP:CZ3	1:B:900:LEU:HB3	2.38	0.58
1:B:451:TYR:O	1:B:464:TRP:NE1	2.35	0.58
1:B:212:LEU:HD12	1:B:246:LEU:HD21	1.84	0.58
1:B:8:GLY:HA3	1:B:991:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1216:SER:OG	1:B:1217:ALA:N	2.36	0.58
1:B:849:ASP:HB3	1:B:854:ASN:HD22	1.69	0.58
1:B:170:ILE:O	1:B:413:GLN:NE2	2.37	0.57
1:B:1321:PRO:O	1:B:1333:ARG:HD2	2.04	0.57
1:B:672:ASP:HB3	1:B:675:SER:HB2	1.85	0.57
1:B:226:ILE:HG22	1:B:242:ILE:HD11	1.87	0.57
1:B:1114:ARG:NH1	4:D:25:DG:OP1	2.38	0.57
1:B:1158:LYS:HE2	1:B:1159:SER:H	1.70	0.57
1:B:764:ALA:HB3	1:B:925:ARG:HG2	1.88	0.56
1:B:100:ARG:NH2	1:B:118:ILE:O	2.37	0.56
1:B:737:ILE:HG13	1:B:927:ILE:HG13	1.87	0.56
1:B:129:HIS:CE1	2:A:27:G:H1'	2.41	0.56
1:B:682:PHE:HB3	1:B:696:LEU:HD21	1.87	0.56
1:B:499:ASP:OD2	1:B:663:SER:N	2.29	0.56
1:B:206:VAL:HG11	1:B:228:GLN:HG3	1.88	0.55
1:B:1220:LEU:HD21	1:B:1342:VAL:HG21	1.88	0.55
1:B:184:LEU:O	1:B:188:LEU:HB2	2.07	0.55
1:B:144:ASP:OD1	1:B:313:THR:OG1	2.20	0.55
1:B:212:LEU:HB3	1:B:300:ILE:HD11	1.89	0.55
1:B:559:VAL:O	1:B:587:PHE:HD1	1.89	0.55
1:B:475:PRO:HG3	2:A:77:U:O4	2.07	0.55
2:A:95:A:H2'	2:A:96:A:C8	2.41	0.55
1:B:258:LEU:HG	1:B:260:GLU:H	1.72	0.55
1:B:870:VAL:HG12	1:B:903:ALA:HB2	1.88	0.54
1:B:644:ASP:HB3	1:B:647:VAL:HG23	1.90	0.54
1:B:100:ARG:HA	1:B:103:GLU:HG2	1.89	0.54
2:A:102:A:H61	2:A:112:U:H3	1.56	0.54
1:B:31:LYS:HA	1:B:44:LYS:HA	1.90	0.54
1:B:148:LYS:HB2	1:B:429:PHE:CE1	2.43	0.54
3:C:16:DT:C4	3:C:17:DC:C5	2.96	0.54
1:B:812:TYR:O	1:B:816:LEU:HB2	2.08	0.53
1:B:502:LEU:HD13	1:B:666:LEU:HD13	1.90	0.53
1:B:1177:ASN:HB3	1:B:1180:ASP:OD1	2.08	0.53
1:B:18:TRP:CZ2	1:B:1353:THR:HB	2.43	0.53
1:B:1147:ALA:HB2	1:B:1190:VAL:HG22	1.91	0.53
1:B:1311:HIS:O	1:B:1314:THR:HG22	2.08	0.53
1:B:527:VAL:HA	1:B:582:GLY:HA3	1.91	0.53
3:C:12:DC:H2'	3:C:13:DG:H8	1.72	0.53
2:A:88:C:H5	2:A:97:G:H1	1.56	0.53
2:A:40:U:H1'	2:A:48:A:C2	2.44	0.53
1:B:1283:ALA:HB1	1:B:1286:ASN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:976:ARG:HG2	1:B:982:HIS:CD2	2.43	0.53
1:B:288:ASP:O	1:B:291:LEU:HG	2.08	0.53
1:B:515:TYR:HE1	1:B:662:LEU:HB2	1.74	0.53
1:B:313:THR:OG1	1:B:314:LYS:N	2.42	0.52
1:B:317:LEU:HD21	1:B:410:ILE:HD13	1.90	0.52
1:B:584:GLU:O	1:B:586:ARG:N	2.42	0.52
3:C:17:DC:H2'	3:C:18:DA:C8	2.45	0.52
1:B:291:LEU:O	1:B:295:ASN:ND2	2.43	0.52
1:B:279:LEU:O	1:B:283:GLY:N	2.42	0.52
1:B:735:LYS:O	1:B:739:GLN:HG2	2.08	0.52
1:B:811:LEU:HD23	1:B:833:LEU:HD11	1.90	0.52
1:B:1022:ILE:O	1:B:1024:LYS:N	2.42	0.52
1:B:76:LYS:NZ	1:B:102:GLU:OE2	2.41	0.52
1:B:1224:ASN:HB2	1:B:1280:VAL:HG11	1.91	0.52
3:C:5:DT:H2''	3:C:6:DC:H5'	1.92	0.52
1:B:720:LEU:CD1	1:B:938:ARG:HH21	2.23	0.51
1:B:814:TYR:CE1	1:B:819:GLY:HA2	2.45	0.51
2:A:31:U:H2'	2:A:32:A:C8	2.46	0.51
1:B:70:ARG:HD3	2:A:79:C:OP2	2.11	0.51
1:B:736:GLY:HA3	1:B:927:ILE:HD12	1.93	0.51
1:B:883:TRP:CE3	1:B:900:LEU:HB3	2.46	0.51
1:B:338:LEU:HB3	1:B:383:MET:HE2	1.93	0.51
1:B:944:ASP:OD1	1:B:948:LYS:N	2.41	0.51
3:C:17:DC:H2'	3:C:18:DA:H8	1.76	0.51
1:B:770:THR:CG2	1:B:1032:ALA:HB3	2.39	0.51
1:B:628:ASP:OD1	1:B:631:MET:HG3	2.11	0.50
2:A:95:A:H2'	2:A:96:A:H8	1.76	0.50
1:B:821:ASP:HB2	1:B:828:LEU:HD21	1.92	0.50
1:B:1061:PRO:HG2	1:B:1064:GLU:HG2	1.93	0.50
1:B:1099:GLU:HB2	2:A:85:C:N4	2.25	0.50
1:B:1198:LEU:HD21	1:B:1347:LEU:HD11	1.93	0.50
1:B:289:LEU:HD12	1:B:289:LEU:H	1.77	0.50
1:B:977:GLU:H	1:B:977:GLU:CD	2.12	0.50
1:B:556:ASN:HB2	1:B:559:VAL:HG22	1.94	0.50
1:B:167:HIS:CE1	1:B:411:PRO:HB3	2.47	0.49
1:B:132:TYR:OH	1:B:141:LYS:HG2	2.13	0.49
4:D:18:DC:H2''	4:D:19:DG:C5	2.48	0.49
1:B:876:VAL:HG21	1:B:903:ALA:HB3	1.95	0.49
1:B:781:MET:HG2	1:B:803:ASN:CB	2.41	0.49
1:B:869:ASN:HD21	1:B:908:LEU:H	1.59	0.49
1:B:13:THR:HG23	1:B:924:THR:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ARG:HD3	1:B:163:LYS:HG3	1.95	0.49
1:B:1006:SER:OG	1:B:1014:LYS:N	2.44	0.49
1:B:148:LYS:HB2	1:B:429:PHE:CD1	2.48	0.49
1:B:175:ASN:O	1:B:177:ASP:N	2.46	0.49
1:B:1061:PRO:HG2	1:B:1064:GLU:HA	1.95	0.49
3:C:5:DT:H2''	3:C:6:DC:C5'	2.43	0.49
2:A:40:U:H1'	2:A:48:A:H2	1.78	0.49
1:B:631:MET:O	1:B:635:ARG:HG2	2.12	0.49
1:B:1085:LYS:O	1:B:1089:MET:HG3	2.13	0.48
1:B:386:THR:HG1	1:B:387:GLU:H	1.57	0.48
1:B:737:ILE:CG1	1:B:927:ILE:HG13	2.43	0.48
1:B:767:ASN:N	1:B:767:ASN:OD1	2.47	0.48
1:B:569:PHE:O	1:B:574:CYS:N	2.46	0.48
1:B:860:SER:OG	1:B:863:ASN:OD1	2.26	0.48
1:B:302:LEU:HD13	1:B:305:ILE:O	2.14	0.48
1:B:1136:SER:HA	4:D:23:DG:O3'	2.14	0.48
2:A:112:U:H2'	2:A:113:G:H8	1.78	0.48
1:B:1139:VAL:HA	1:B:1167:THR:HA	1.96	0.48
1:B:1307:GLU:O	1:B:1310:ILE:HB	2.14	0.48
1:B:170:ILE:HG21	1:B:174:LEU:HD21	1.95	0.48
1:B:185:PHE:O	1:B:189:VAL:HG23	2.14	0.48
1:B:7:ILE:HG12	1:B:20:VAL:HG22	1.95	0.48
1:B:823:TYR:OH	1:B:839:ASP:OD2	2.20	0.48
1:B:1006:SER:O	1:B:1013:TYR:HA	2.15	0.47
1:B:305:ILE:HG21	1:B:317:LEU:HD12	1.96	0.47
1:B:386:THR:O	1:B:388:GLU:N	2.48	0.47
1:B:244:LEU:HB2	1:B:250:PRO:HG2	1.94	0.47
1:B:770:THR:HG23	1:B:1033:THR:H	1.78	0.47
1:B:1096:LYS:HE3	1:B:1201:TYR:CE2	2.49	0.47
1:B:7:ILE:HD13	1:B:747:LEU:CD1	2.45	0.47
1:B:403:ARG:NH1	2:A:20:C:OP2	2.48	0.47
1:B:1281:ILE:HD11	1:B:1316:THR:HA	1.97	0.47
1:B:556:ASN:O	1:B:595:HIS:NE2	2.48	0.47
1:B:957:THR:O	1:B:957:THR:OG1	2.33	0.47
1:B:65:LYS:NZ	1:B:1108:GLU:OE2	2.46	0.47
1:B:116:HIS:HA	1:B:117:PRO:HD3	1.71	0.47
1:B:762:GLU:OE2	1:B:960:SER:HA	2.15	0.47
1:B:824:VAL:HG22	1:B:863:ASN:HD22	1.79	0.47
1:B:275:LEU:HD21	1:B:290:PHE:HD1	1.80	0.47
1:B:658:GLY:C	1:B:659:TRP:CD1	2.89	0.47
1:B:104:SER:O	2:A:25:U:H1'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1326:TYR:CE2	1:B:1327:PHE:HD2	2.34	0.46
1:B:297:SER:O	1:B:300:ILE:HG22	2.15	0.46
1:B:501:ASN:O	1:B:503:PRO:HD3	2.15	0.46
2:A:53:C:O5'	2:A:53:C:H6	1.98	0.46
1:B:318:SER:OG	1:B:418:GLU:OE1	2.29	0.46
1:B:1236:LEU:HA	1:B:1236:LEU:HD23	1.73	0.46
1:B:564:LEU:O	1:B:568:TYR:HB3	2.16	0.46
1:B:672:ASP:O	1:B:676:GLY:N	2.49	0.46
1:B:1086:VAL:HA	1:B:1089:MET:SD	2.55	0.46
1:B:144:ASP:CG	1:B:313:THR:HG1	2.16	0.46
1:B:568:TYR:HD2	1:B:569:PHE:CD2	2.34	0.46
4:D:15:DA:H4'	4:D:16:DG:OP1	2.16	0.46
1:B:544:GLN:O	1:B:548:ILE:HG12	2.15	0.46
1:B:549:VAL:HG21	1:B:684:LYS:NZ	2.30	0.46
1:B:1075:ASP:OD2	1:B:1078:ARG:N	2.49	0.46
1:B:1161:LYS:HE2	1:B:1343:LEU:HB3	1.98	0.46
1:B:530:VAL:HG22	1:B:537:PRO:HA	1.97	0.46
1:B:499:ASP:HB2	1:B:663:SER:HB2	1.97	0.46
3:C:27:DC:C4	3:C:28:DG:N7	2.84	0.46
1:B:225:LEU:HA	1:B:225:LEU:HD13	1.78	0.46
1:B:5:TYR:CZ	1:B:751:MET:HB3	2.51	0.46
1:B:1326:TYR:CD2	1:B:1327:PHE:HD2	2.33	0.45
3:C:3:DA:H61	4:D:28:DT:H3	1.64	0.45
2:A:5:C:H2'	2:A:6:A:H8	1.80	0.45
1:B:1303:ARG:HB3	1:B:1303:ARG:CZ	2.46	0.45
1:B:260:GLU:OE2	1:B:557:ARG:HG3	2.17	0.45
2:A:3:C:C2	2:A:4:G:N7	2.84	0.45
1:B:224:ASN:N	1:B:224:ASN:OD1	2.49	0.45
1:B:1121:ALA:HB1	1:B:1123:LYS:O	2.17	0.45
1:B:614:ASP:HA	1:B:664:ARG:HH22	1.80	0.45
1:B:977:GLU:HG3	1:B:1310:ILE:HG23	1.97	0.45
1:B:597:LEU:O	1:B:601:ILE:HG13	2.16	0.45
1:B:924:THR:HA	1:B:927:ILE:HG22	1.98	0.45
1:B:1207:GLU:OE2	1:B:1210:ARG:NH1	2.50	0.45
1:B:157:ALA:O	1:B:161:MET:HG3	2.17	0.45
2:A:72:G:C6	2:A:73:C:N4	2.85	0.44
1:B:48:ILE:HG12	1:B:984:ALA:HB1	1.99	0.44
3:C:12:DC:H2'	3:C:13:DG:C8	2.51	0.44
1:B:35:LEU:HB3	1:B:36:GLY:H	1.65	0.44
1:B:151:LEU:HD11	1:B:432:PHE:HZ	1.81	0.44
1:B:784:ILE:O	1:B:788:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ARG:HH11	2:A:18:C:P	2.40	0.44
1:B:502:LEU:HD11	1:B:670:ILE:HD11	1.99	0.44
1:B:816:LEU:HD23	1:B:891:LEU:HB3	1.99	0.44
1:B:156:LEU:HD23	1:B:156:LEU:HA	1.78	0.44
1:B:516:GLU:HB3	1:B:591:LEU:HD23	1.99	0.44
1:B:894:GLN:HG2	1:B:895:ARG:N	2.33	0.44
1:B:251:ASN:ND2	1:B:261:ASP:OD1	2.38	0.44
1:B:468:LYS:N	1:B:481:VAL:O	2.47	0.44
1:B:788:ILE:HG13	1:B:796:LEU:HD13	2.00	0.44
4:D:13:DT:H2''	4:D:14:DG:O4'	2.18	0.44
4:D:23:DG:H2''	4:D:24:DC:O4'	2.17	0.44
2:A:64:A:H2'	2:A:65:A:C8	2.52	0.44
1:B:733:ILE:HG23	1:B:927:ILE:HB	2.00	0.44
1:B:108:GLU:OE2	1:B:115:ARG:HD3	2.17	0.44
1:B:1208:ASN:O	1:B:1279:ARG:NH1	2.51	0.44
1:B:1326:TYR:CE2	1:B:1327:PHE:CD2	3.06	0.44
1:B:342:GLN:HB2	1:B:383:MET:HE3	2.00	0.44
1:B:763:MET:HG3	1:B:957:THR:HB	2.00	0.44
1:B:448:ILE:HD13	1:B:455:LEU:HD13	2.00	0.43
1:B:917:ILE:HG12	1:B:920:GLN:HG3	1.99	0.43
1:B:1351:SER:HA	2:A:86:A:C5	2.53	0.43
4:D:15:DA:H2''	4:D:16:DG:C8	2.53	0.43
1:B:1351:SER:HA	2:A:86:A:N7	2.32	0.43
1:B:1183:GLU:HA	1:B:1187:TYR:O	2.18	0.43
1:B:764:ALA:CB	1:B:925:ARG:HE	2.31	0.43
1:B:1111:LEU:HA	1:B:1112:PRO:HD3	1.86	0.43
1:B:378:PRO:HA	1:B:381:GLU:HG2	2.00	0.43
2:A:112:U:H2'	2:A:113:G:C8	2.52	0.43
2:A:82:U:O5'	2:A:82:U:H6	2.00	0.43
1:B:893:THR:OG1	1:B:894:GLN:N	2.52	0.43
1:B:8:GLY:CA	1:B:991:ALA:HB2	2.49	0.43
1:B:90:MET:HE3	1:B:151:LEU:HD23	1.99	0.43
1:B:601:ILE:HG22	1:B:647:VAL:HG11	2.00	0.43
2:A:110:G:H2'	2:A:111:G:C8	2.53	0.43
1:B:345:GLU:H	1:B:345:GLU:CD	2.21	0.43
1:B:480:GLU:OE1	1:B:480:GLU:N	2.51	0.43
1:B:1113:LYS:HE3	2:A:24:U:H5'	2.00	0.43
1:B:1221:GLN:HG2	1:B:1320:ALA:HA	2.01	0.43
1:B:746:GLU:OE2	1:B:1353:THR:OG1	2.19	0.43
1:B:981:TYR:CE1	1:B:1092:VAL:HB	2.54	0.43
1:B:137:HIS:HA	1:B:322:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:SER:HB3	1:B:220:ARG:CB	2.49	0.43
1:B:816:LEU:O	1:B:891:LEU:HD13	2.19	0.43
1:B:188:LEU:O	1:B:191:THR:OG1	2.26	0.42
1:B:560:THR:HG23	1:B:563:GLN:H	1.84	0.42
1:B:666:LEU:HD12	1:B:666:LEU:HA	1.75	0.42
1:B:666:LEU:HD12	1:B:670:ILE:HD12	2.01	0.42
1:B:813:LEU:HD21	1:B:852:ILE:HG23	2.00	0.42
3:C:26:DG:O5'	3:C:26:DG:H8	2.02	0.42
2:A:29:G:N2	2:A:59:A:H1'	2.34	0.42
1:B:1065:THR:HA	1:B:1073:VAL:HG22	2.01	0.42
1:B:1200:LYS:HE2	1:B:1201:TYR:CE1	2.54	0.42
4:D:18:DC:C6	4:D:18:DC:H5"	2.54	0.42
1:B:1349:HIS:HB3	2:A:86:A:N3	2.34	0.42
1:B:667:ILE:HD13	1:B:667:ILE:HG21	1.75	0.42
1:B:531:THR:HG23	1:B:575:PHE:CD2	2.53	0.42
1:B:624:THR:HA	1:B:656:TYR:O	2.19	0.42
1:B:770:THR:HG23	1:B:1033:THR:OG1	2.19	0.42
1:B:1266:LEU:O	1:B:1270:ILE:HG12	2.19	0.42
1:B:167:HIS:HB2	1:B:169:LEU:HG	2.01	0.42
1:B:338:LEU:HB3	1:B:383:MET:CE	2.48	0.42
1:B:682:PHE:CE1	1:B:702:LEU:HD11	2.54	0.42
1:B:788:ILE:HG13	1:B:796:LEU:CD1	2.50	0.42
1:B:900:LEU:HA	1:B:900:LEU:HD23	1.82	0.42
1:B:756:PRO:O	1:B:953:VAL:HG22	2.20	0.42
1:B:305:ILE:HG23	1:B:321:MET:HE3	2.02	0.42
1:B:993:VAL:O	1:B:997:LEU:HB2	2.20	0.42
1:B:1255:LYS:O	1:B:1259:VAL:HG23	2.19	0.42
1:B:698:HIS:ND1	3:C:30:DC:H2"	2.35	0.42
1:B:133:PRO:HG2	1:B:137:HIS:CE1	2.55	0.41
1:B:661:ARG:HG3	2:A:5:C:OP2	2.19	0.41
2:A:22:U:H2'	2:A:23:U:C6	2.54	0.41
2:A:29:G:H21	2:A:59:A:H1'	1.85	0.41
1:B:122:ILE:O	1:B:126:VAL:HG23	2.20	0.41
1:B:70:ARG:NH2	2:A:15:A:OP1	2.51	0.41
2:A:27:G:H4'	2:A:28:A:OP2	2.20	0.41
1:B:1207:GLU:HB2	1:B:1208:ASN:H	1.57	0.41
1:B:735:LYS:HA	2:A:84:U:OP1	2.21	0.41
2:A:64:A:C2	2:A:65:A:C4	3.08	0.41
1:B:829:ASP:OD1	1:B:830:ILE:N	2.53	0.41
1:B:995:THR:O	1:B:998:ILE:HG13	2.20	0.41
1:B:525:THR:OG1	1:B:690:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:LEU:CD1	1:B:659:TRP:HH2	2.34	0.41
2:A:102:A:C6	2:A:113:G:C6	3.08	0.41
1:B:997:LEU:HA	1:B:997:LEU:HD23	1.81	0.41
2:A:69:A:C2	2:A:80:G:H2'	2.55	0.41
1:B:507:VAL:HG11	1:B:660:GLY:O	2.21	0.41
3:C:27:DC:N4	3:C:28:DG:N7	2.69	0.41
2:A:4:G:H2'	2:A:5:C:H6	1.82	0.41
1:B:27:VAL:HA	1:B:28:PRO:HD3	1.88	0.41
1:B:560:THR:HG23	1:B:563:GLN:HB2	2.03	0.41
1:B:615:ILE:HG23	1:B:639:TYR:CZ	2.56	0.41
1:B:71:ARG:HD3	2:A:18:C:OP2	2.21	0.41
1:B:1287:LEU:O	1:B:1291:LEU:HG	2.22	0.41
1:B:642:LEU:HA	1:B:642:LEU:HD23	1.68	0.41
1:B:694:MET:HB2	3:C:29:DC:H1'	2.03	0.41
3:C:4:DA:C2	3:C:5:DT:C2	3.08	0.41
1:B:70:ARG:HH11	2:A:79:C:P	2.43	0.40
1:B:740:THR:HG21	1:B:931:VAL:HG21	2.03	0.40
1:B:1110:ILE:HB	2:A:22:U:O2'	2.20	0.40
1:B:1158:LYS:HD2	1:B:1158:LYS:HA	1.73	0.40
1:B:522:ASN:O	1:B:525:THR:HG22	2.22	0.40
1:B:626:PHE:CD2	1:B:631:MET:HE1	2.56	0.40
1:B:682:PHE:CB	1:B:696:LEU:HD21	2.51	0.40
1:B:787:GLY:HA3	1:B:891:LEU:HD21	2.02	0.40
2:A:17:A:C2	2:A:18:C:C2	3.09	0.40
1:B:973:TYR:HB3	1:B:1237:TYR:CD2	2.57	0.40
1:B:601:ILE:H	1:B:601:ILE:HG13	1.65	0.40
1:B:849:ASP:OD1	1:B:851:SER:OG	2.23	0.40
1:B:88:ASN:N	1:B:88:ASN:OD1	2.44	0.40
1:B:549:VAL:HA	1:B:553:PHE:HB2	2.02	0.40
1:B:7:ILE:HD13	1:B:747:LEU:HD13	2.04	0.40
1:B:25:TYR:CE1	1:B:996:ALA:HB2	2.57	0.40
4:D:17:DA:H5'	4:D:17:DA:H8	1.82	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	B	1360/1368 (99%)	1247 (92%)	91 (7%)	22 (2%)	12 53

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	177	ASP
1	B	711	ALA
1	B	1029	ILE
1	B	1208	ASN
1	B	308	VAL
1	B	387	GLU
1	B	669	GLY
1	B	722	GLU
1	B	831	ASN
1	B	1023	ALA
1	B	1031	LYS
1	B	1284	ASP
1	B	210	ALA
1	B	582	GLY
1	B	585	ASP
1	B	1032	ALA
1	B	176	PRO
1	B	1056	GLU
1	B	1245	LEU
1	B	285	GLN
1	B	871	PRO
1	B	717	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	994/1227 (81%)	953 (96%)	41 (4%)	37 75

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	THR
1	B	71	ARG
1	B	88	ASN
1	B	90	MET
1	B	165	ARG
1	B	188	LEU
1	B	216	LEU
1	B	278	LEU
1	B	282	ILE
1	B	288	ASP
1	B	302	LEU
1	B	305	ILE
1	B	334	LEU
1	B	390	LEU
1	B	403	ARG
1	B	437	ARG
1	B	465	MET
1	B	548	ILE
1	B	555	THR
1	B	560	THR
1	B	564	LEU
1	B	578	VAL
1	B	614	ASP
1	B	625	LEU
1	B	726	ASN
1	B	740	THR
1	B	767	ASN
1	B	816	LEU
1	B	830	ILE
1	B	847	LEU
1	B	917	ILE
1	B	1026	GLU
1	B	1084	ARG
1	B	1158	LYS
1	B	1179	ILE

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Mol	Chain	Res	Type
1	B	1207	GLU
1	B	1240	SER
1	B	1242	TYR
1	B	1248	SER
1	B	1272	GLN
1	B	1284	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	668	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	114/118 (96%)	25 (21%)	6 (5%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	9	A
2	A	11	G
2	A	17	A
2	A	20	C
2	A	24	U
2	A	28	A
2	A	29	G
2	A	38	U
2	A	41	U
2	A	45	A
2	A	48	A
2	A	49	A
2	A	50	C
2	A	60	A
2	A	61	G
2	A	69	A
2	A	74	U
2	A	77	U
2	A	86	A
2	A	87	A

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Mol	Chain	Res	Type
2	A	92	A
2	A	105	G
2	A	107	G
2	A	109	C
2	A	116	U

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	8	A
2	A	27	G
2	A	47	A
2	A	49	A
2	A	60	A
2	A	86	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	A	201	-	4,4,4	0.19	0	6,6,6	0.20	0
5	SO4	B	1401	-	4,4,4	0.19	0	6,6,6	0.33	0
5	SO4	C	101	-	4,4,4	0.34	0	6,6,6	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	201	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1401	-	-	0/0/0/0	0/0/0/0
5	SO4	C	101	-	-	0/0/0/0	0/0/0/0

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(Å ²)	Q<0.9
1	B	1362/1368 (99%)	0.36	69 (5%) 32 28	59, 128, 192, 261	0
2	A	115/118 (97%)	0.54	11 (9%) 10 10	56, 128, 293, 312	0
3	C	30/30 (100%)	-0.07	0 100 100	57, 82, 142, 149	0
4	D	19/30 (63%)	-0.23	0 100 100	60, 102, 165, 199	0
All	All	1526/1546 (98%)	0.36	80 (5%) 31 28	56, 128, 198, 312	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	49	A	5.0
1	B	47	LEU	4.9
1	B	32	PHE	4.5
1	B	578	VAL	4.5
2	A	47	A	4.2
1	B	576	ASP	4.0
1	B	286	TYR	3.9
2	A	48	A	3.9
1	B	683	LEU	3.9
1	B	1028	GLU	3.9
2	A	46	A	3.4
2	A	50	C	3.4
2	A	40	U	3.3
1	B	1355	LEU	3.2
1	B	1025	SER	3.2
1	B	48	ILE	3.2
1	B	1359	ARG	3.2
2	A	42	G	3.1
1	B	524	LEU	3.1
1	B	600	ILE	3.1
1	B	402	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	998	ILE	3.0
1	B	1126	TRP	3.0
1	B	1145	VAL	3.0
1	B	580	ILE	2.9
1	B	310	THR	2.9
2	A	41	U	2.9
1	B	693	PHE	2.8
1	B	679	ILE	2.8
1	B	551	LEU	2.8
1	B	1315	LEU	2.8
1	B	577	SER	2.8
1	B	1235	PHE	2.7
1	B	46	ASN	2.7
1	B	768	GLN	2.7
1	B	815	TYR	2.7
1	B	266	LEU	2.7
1	B	806	LEU	2.7
2	A	37	G	2.7
1	B	594	TYR	2.6
1	B	1027	GLN	2.6
1	B	690	ASN	2.6
1	B	154	ILE	2.6
1	B	174	LEU	2.6
1	B	1157	LEU	2.6
1	B	86	PHE	2.5
1	B	198	GLU	2.5
1	B	540	LEU	2.5
1	B	305	ILE	2.5
1	B	988	TYR	2.5
1	B	1203	LEU	2.4
1	B	1022	ILE	2.4
1	B	128	TYR	2.4
1	B	1357	GLU	2.4
1	B	1090	PRO	2.4
1	B	226	ILE	2.4
1	B	981	TYR	2.4
2	A	45	A	2.4
1	B	583	VAL	2.4
1	B	527	VAL	2.3
1	B	640	ALA	2.3
1	B	1050	ILE	2.3
1	B	1134	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1093	ASN	2.3
2	A	39	U	2.3
1	B	1149	VAL	2.2
1	B	289	LEU	2.2
1	B	1125	ASP	2.2
1	B	317	LEU	2.1
1	B	639	TYR	2.1
1	B	689	ALA	2.1
1	B	195	LEU	2.1
1	B	667	ILE	2.1
1	B	151	LEU	2.1
1	B	1356	TYR	2.1
1	B	553	PHE	2.1
1	B	579	GLU	2.1
1	B	1204	PHE	2.1
1	B	980	ASN	2.0
1	B	582	GLY	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	A	201	5/5	0.87	0.39	1.74	93,110,127,147	0
5	SO4	C	101	5/5	0.92	0.20	0.16	69,94,127,134	0
5	SO4	B	1401	5/5	0.94	0.14	-1.15	92,115,128,141	0

6.5 Other polymers [i](#)

There are no such residues in this entry.