



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2025 – 04:41 PM JST

PDB ID : 9L9W
Title : Structure of SPARTA in complex with guide DNA and a 19nt target DNA
Authors : Hu, R.; Guo, C.; Liu, X.; Chen, J.; Liu, L.
Deposited on : 2024-12-31
Resolution : 5.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

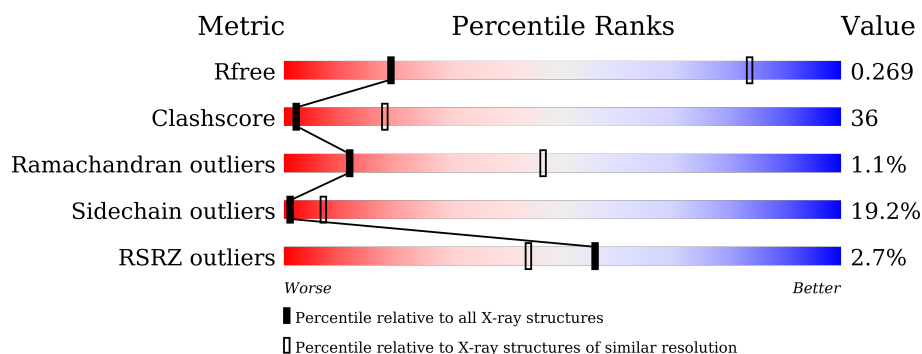
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.87 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}	164625	1071 (7.76-4.00)
Clashscore	180529	1112 (7.76-4.00)
Ramachandran outliers	177936	1003 (7.70-3.98)
Sidechain outliers	177891	1012 (7.80-3.96)
RSRZ outliers	164620	1066 (7.76-4.00)

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	507	<div> <div>2%</div> <div> <div></div> <div>35%</div> <div>50%</div> <div>8%</div> <div>7%</div> </div> </div>
2	B	421	<div> <div>3%</div> <div> <div></div> <div>36%</div> <div>50%</div> <div>12%</div> </div> </div>
3	C	21	<div> <div>10%</div> <div> <div></div> <div>48%</div> <div>43%</div> </div> </div>
4	D	20	<div> <div>10%</div> <div> <div></div> <div>55%</div> <div>40%</div> <div>5%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8099 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 Piwi domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3827	2479	636	700	12			

- Molecule 2 is a protein called TIR domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3452	2239	579	623	11			

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*AP*TP*AP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	21	Total	C	N	O	P	0	0	0
			442	210	81	130	21			

- Molecule 4 is a DNA chain called DNA (5'-D(*T*AP*TP*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*CP*TP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	19	Total	C	N	O	P	0	0	0
			377	183	66	110	18			

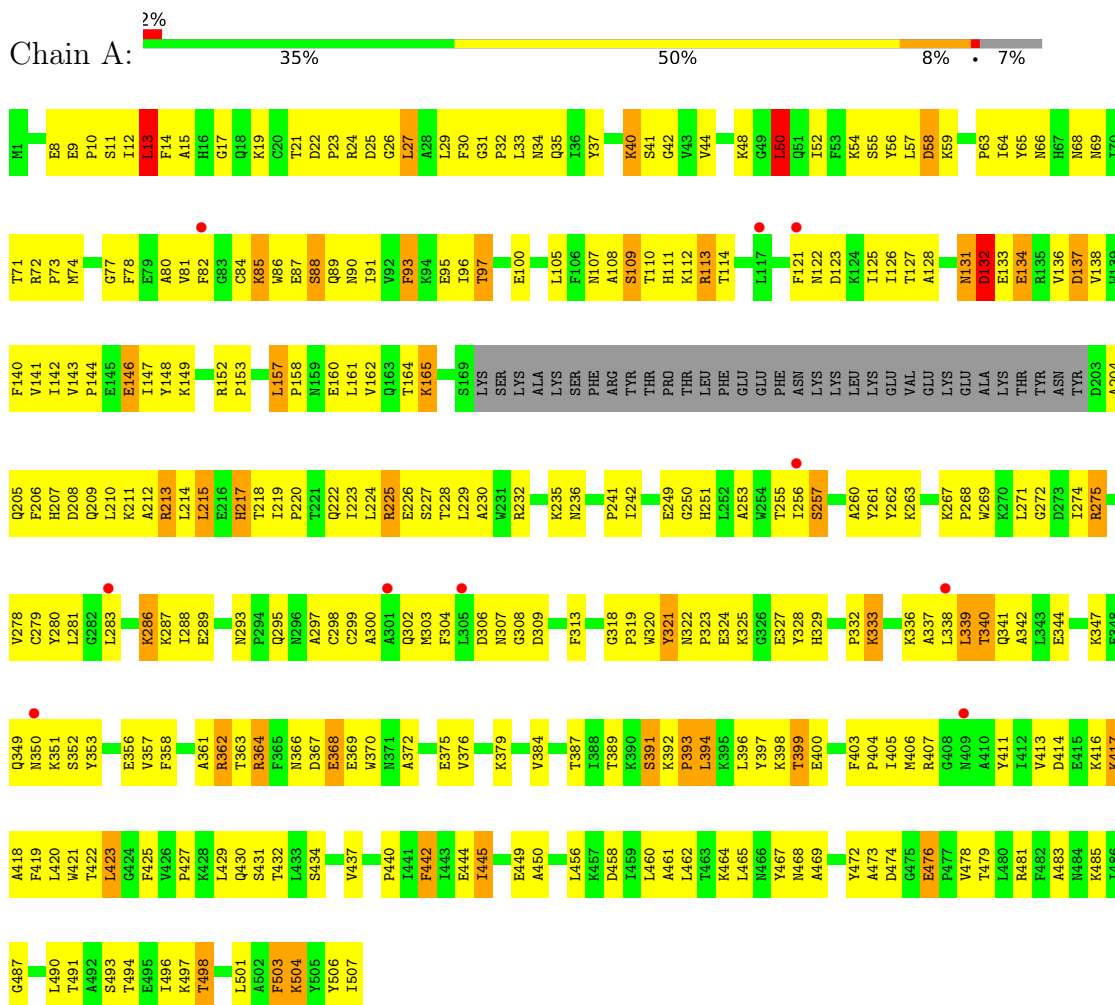
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		

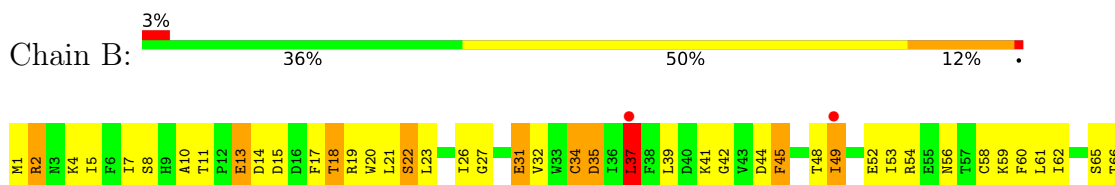
3 Residue-property plots

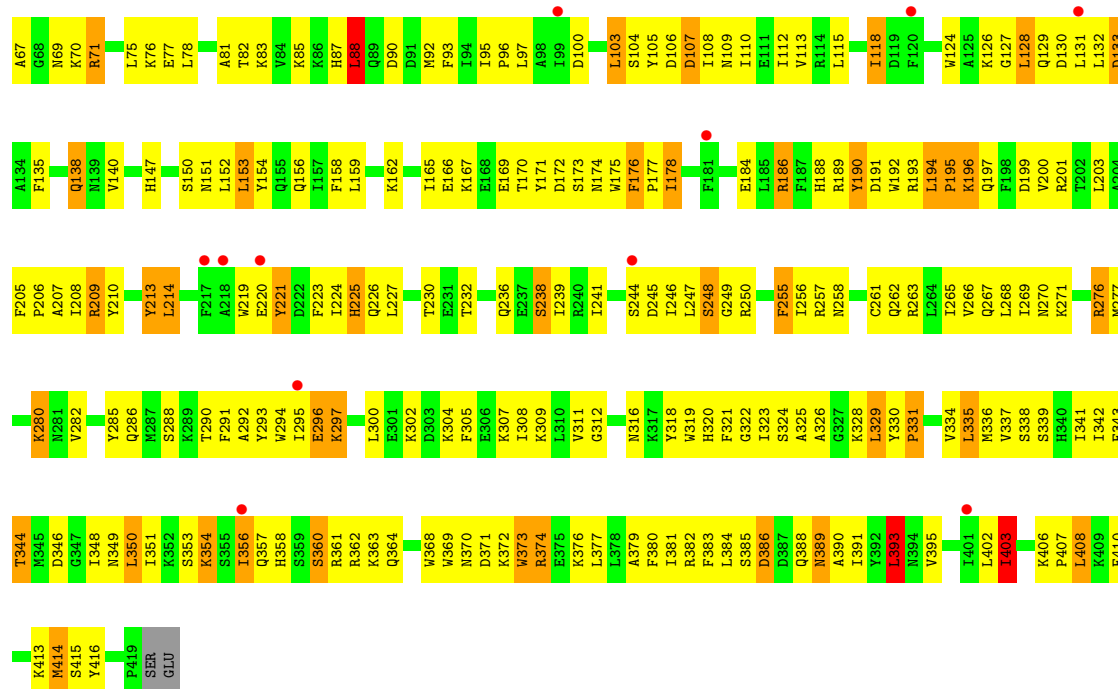
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

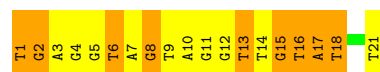


• Molecule 2: TIR domain-containing protein

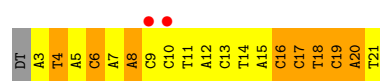




- Molecule 3: DNA (5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*T
P*AP*TP*AP*GP*T)-3')



- Molecule 4: DNA (5'-D(*T*AP*TP*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*CP*T
P*CP*AP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.19Å 136.19Å 174.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.31 – 5.87 39.31 – 5.87	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.31-5.87) 98.4 (39.31-5.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 5.71Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.261 , 0.288 0.244 , 0.269	Depositor DCC
R_{free} test set	266 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	295.2	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 680.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	8099	wwPDB-VP
Average B, all atoms (Å ²)	317.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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

5.1 Standard geometry

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

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	0.68	1/3923 (0.0%)	0.76	3/5313 (0.1%)
2	B	0.79	4/3539 (0.1%)	0.89	10/4780 (0.2%)
3	C	1.77	9/496 (1.8%)	1.40	6/765 (0.8%)
4	D	1.73	9/421 (2.1%)	1.32	2/645 (0.3%)
All	All	0.90	23/8379 (0.3%)	0.91	21/11503 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	360	SER	CB-OG	-15.42	1.22	1.42
3	C	1	DT	OP3-P	-10.60	1.48	1.61
3	C	1	DT	C1'-N1	9.50	1.61	1.49
3	C	17	DA	N9-C4	8.99	1.43	1.37
3	C	2	DG	N9-C8	8.73	1.44	1.37
4	D	18	DT	N1-C6	-8.19	1.32	1.38
4	D	4	DT	C1'-N1	7.64	1.59	1.49
3	C	16	DT	C3'-O3'	7.35	1.53	1.44
4	D	18	DT	C5-C6	-7.27	1.29	1.34
4	D	6	DC	C1'-N1	6.97	1.58	1.49
4	D	18	DT	C2-O2	6.66	1.27	1.22
4	D	8	DA	C3'-O3'	6.66	1.52	1.44
3	C	21	DT	C1'-N1	6.00	1.57	1.49
3	C	15	DG	C3'-O3'	5.53	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	176	PHE	CE2-CZ	-5.50	1.26	1.37
3	C	6	DT	C1'-N1	5.48	1.56	1.49
2	B	42	GLY	CA-C	-5.47	1.43	1.51
1	A	50	LEU	CG-CD2	5.31	1.71	1.51
4	D	19	DC	C1'-N1	5.27	1.56	1.49
3	C	13	DT	C3'-O3'	5.20	1.50	1.44
4	D	17	DC	C1'-N1	-5.12	1.40	1.47
4	D	16	DC	C3'-O3'	-5.10	1.37	1.44
2	B	403	ILE	CB-CG2	5.04	1.68	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	276	ARG	NE-CZ-NH1	9.27	124.93	120.30
2	B	276	ARG	NE-CZ-NH2	-9.08	115.76	120.30
2	B	335	LEU	CA-CB-CG	-8.86	94.93	115.30
1	A	132	ASP	CB-CG-OD2	8.28	125.75	118.30
2	B	176	PHE	CG-CD1-CE1	-7.04	113.06	120.80
3	C	16	DT	P-O3'-C3'	6.17	127.11	119.70
1	A	13	LEU	CA-CB-CG	6.00	129.09	115.30
3	C	8	DG	O4'-C4'-C3'	-5.78	102.19	104.50
2	B	329	LEU	CA-CB-CG	5.58	128.13	115.30
3	C	16	DT	O5'-P-OP1	-5.53	100.73	105.70
2	B	88	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	93	PHE	CB-CG-CD2	-5.48	116.96	120.80
3	C	2	DG	O4'-C1'-N9	5.36	111.75	108.00
4	D	18	DT	C5-C4-O4	-5.31	121.18	124.90
3	C	15	DG	O4'-C1'-N9	5.14	111.60	108.00
2	B	393	LEU	CB-CG-CD1	5.13	119.73	111.00
2	B	118	ILE	CG1-CB-CG2	-5.12	100.13	111.40
3	C	18	DT	N3-C4-O4	5.11	122.97	119.90
2	B	34	CYS	CA-CB-SG	5.10	123.18	114.00
4	D	20	DA	OP2-P-O3'	5.05	116.32	105.20
2	B	37	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	325	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3827	0	3844	270	0
2	B	3452	0	3416	246	0
3	C	442	0	240	41	0
4	D	377	0	216	51	0
5	D	1	0	0	0	0
All	All	8099	0	7716	563	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 36.

All (563) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASN:HD21	1:A:507:ILE:HD13	1.11	1.06
1:A:40:LYS:HG3	1:A:90:ASN:HD21	1.29	0.95
1:A:59:LYS:NZ	1:A:249:GLU:OE1	2.01	0.90
1:A:302:GLN:NE2	1:A:479:THR:O	2.04	0.90
2:B:184:GLU:O	2:B:186:ARG:NH2	2.04	0.90
1:A:9:GLU:OE1	1:A:464:LYS:NZ	2.08	0.87
1:A:268:PRO:HB2	1:A:269:TRP:CE3	2.10	0.86
3:C:12:DG:O6	4:D:9:DC:N4	2.08	0.86
1:A:299:CYS:SG	1:A:300:ALA:N	2.49	0.85
1:A:399:THR:OG1	2:B:170:THR:O	1.94	0.85
2:B:61:LEU:HB3	2:B:97:LEU:HD11	1.59	0.84
3:C:14:DT:H3	4:D:7:DA:H61	1.25	0.84
1:A:468:ASN:HD21	1:A:507:ILE:CD1	1.90	0.83
2:B:65:SER:O	2:B:69:ASN:ND2	2.12	0.82
1:A:344:GLU:OE2	1:A:353:TYR:OH	1.95	0.82
1:A:128:ALA:O	1:A:132:ASP:HB2	1.81	0.81
1:A:262:TYR:OH	1:A:309:ASP:OD1	1.99	0.80
1:A:225:ARG:NE	1:A:227:SER:OG	2.13	0.80
2:B:206:PRO:HG3	2:B:395:VAL:HG12	1.63	0.80
2:B:294:TRP:HZ2	2:B:350:LEU:HD12	1.45	0.80
1:A:327:GLU:OE2	1:A:329:HIS:NE2	2.14	0.80
2:B:294:TRP:CZ2	2:B:350:LEU:HD12	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HH11	2:B:2:ARG:H	1.32	0.78
1:A:468:ASN:ND2	1:A:507:ILE:HD13	1.95	0.78
1:A:153:PRO:HG3	1:A:204:ALA:HB3	1.63	0.77
2:B:265:ILE:O	2:B:269:ILE:HG13	1.82	0.77
2:B:58:CYS:SG	2:B:140:VAL:HG13	2.26	0.76
2:B:282:VAL:HG12	2:B:295:ILE:HG12	1.68	0.76
4:D:15:DA:H2''	4:D:16:DC:H5''	1.68	0.75
1:A:504:LYS:HA	1:A:507:ILE:HD12	1.67	0.75
2:B:81:ALA:O	2:B:85:LYS:N	2.19	0.75
2:B:4:LYS:NZ	2:B:52:GLU:OE1	2.18	0.75
1:A:421:TRP:CE2	1:A:440:PRO:HB3	2.22	0.74
1:A:432:THR:OG1	1:A:434:SER:O	2.04	0.74
1:A:93:PHE:CZ	1:A:95:GLU:HA	2.21	0.74
1:A:275:ARG:NH2	1:A:356:GLU:OE2	2.20	0.74
1:A:389:THR:HG23	1:A:442:PHE:HB3	1.67	0.74
4:D:12:DA:H2''	4:D:13:DC:H5'	1.69	0.74
1:A:421:TRP:NE1	1:A:440:PRO:HD3	2.04	0.73
1:A:108:ALA:HB2	1:A:162:VAL:HG11	1.70	0.73
2:B:320:HIS:NE2	2:B:344:THR:OG1	2.22	0.73
2:B:200:VAL:HA	2:B:203:LEU:HD23	1.71	0.72
1:A:421:TRP:HE1	1:A:440:PRO:HD3	1.55	0.72
2:B:188:HIS:HA	2:B:238:SER:OG	1.89	0.72
4:D:17:DC:H2''	4:D:18:DT:H5''	1.70	0.72
2:B:364:GLN:OE1	2:B:368:TRP:NE1	2.22	0.71
1:A:483:ALA:O	1:A:487:GLY:N	2.23	0.71
2:B:105:TYR:CE1	2:B:113:VAL:HG11	2.25	0.71
2:B:92:MET:HG2	2:B:138:GLN:HE22	1.55	0.71
2:B:132:LEU:O	2:B:135:PHE:N	2.24	0.70
1:A:29:LEU:HB3	1:A:30:PHE:CE1	2.26	0.70
2:B:294:TRP:HB3	2:B:342:ILE:HG13	1.73	0.70
2:B:34:CYS:HB3	2:B:37:LEU:HD22	1.74	0.70
1:A:52:ILE:HD12	1:A:226:GLU:HG2	1.73	0.70
1:A:50:LEU:CD2	1:A:93:PHE:CD2	2.75	0.70
2:B:97:LEU:HD23	2:B:118:ILE:HG21	1.73	0.70
1:A:44:VAL:HG21	1:A:125:ILE:HG12	1.74	0.69
1:A:69:ASN:HA	1:A:72:ARG:O	1.92	0.69
2:B:330:TYR:CD2	2:B:331:PRO:HA	2.27	0.69
2:B:354:LYS:HA	2:B:357:GLN:HB2	1.75	0.68
2:B:199:ASP:OD1	2:B:201:ARG:NH2	2.24	0.68
2:B:203:LEU:HD12	2:B:223:PHE:HD1	1.58	0.68
2:B:173:SER:OG	2:B:175:TRP:N	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:MET:HG2	2:B:138:GLN:NE2	2.08	0.67
3:C:11:DG:N2	4:D:11:DT:O2	2.28	0.67
1:A:257:SER:HA	1:A:260:ALA:HB3	1.74	0.67
1:A:421:TRP:CD2	1:A:440:PRO:HB3	2.30	0.67
2:B:341:ILE:HB	2:B:361:ARG:HD3	1.76	0.67
2:B:209:ARG:HH21	2:B:209:ARG:HB3	1.59	0.67
1:A:283:LEU:HB2	1:A:361:ALA:HB2	1.76	0.67
2:B:97:LEU:HA	2:B:118:ILE:HG22	1.77	0.67
2:B:379:ALA:O	2:B:383:PHE:N	2.27	0.66
4:D:6:DC:H2''	4:D:7:DA:C8	2.30	0.66
1:A:212:ALA:O	1:A:215:LEU:HB2	1.96	0.66
2:B:186:ARG:HG3	2:B:188:HIS:CE1	2.31	0.66
1:A:406:MET:HE3	1:A:427:PRO:HD3	1.77	0.66
1:A:421:TRP:CZ2	1:A:440:PRO:HG3	2.31	0.66
2:B:343:PHE:HB2	2:B:357:GLN:HE21	1.60	0.66
2:B:108:ILE:HB	2:B:113:VAL:HG22	1.78	0.66
2:B:82:THR:HA	2:B:85:LYS:HB2	1.77	0.66
3:C:4:DG:O6	4:D:16:DC:N4	2.28	0.66
1:A:52:ILE:HG23	1:A:230:ALA:HB2	1.77	0.65
2:B:236:GLN:N	2:B:236:GLN:OE1	2.28	0.65
2:B:97:LEU:HA	2:B:118:ILE:CG2	2.26	0.65
2:B:380:PHE:O	2:B:383:PHE:HB3	1.97	0.65
1:A:318:GLY:HA3	1:A:320:TRP:CZ2	2.30	0.65
1:A:143:VAL:HG13	1:A:147:ILE:HB	1.79	0.64
1:A:225:ARG:NH2	1:A:227:SER:OG	2.30	0.64
4:D:20:DA:H4'	4:D:21:DT:OP2	1.97	0.64
2:B:246:ILE:HG21	2:B:261:CYS:SG	2.38	0.64
2:B:147:HIS:O	2:B:150:SER:HB3	1.96	0.64
1:A:122:ASN:HD22	1:A:213:ARG:HG2	1.62	0.64
1:A:391:SER:C	1:A:393:PRO:HD3	2.19	0.64
1:A:257:SER:O	1:A:261:TYR:N	2.18	0.64
2:B:11:THR:HG22	2:B:15:ASP:OD1	1.98	0.64
2:B:44:ASP:O	2:B:48:THR:N	2.15	0.63
1:A:418:ALA:HB3	1:A:456:LEU:HD21	1.81	0.63
3:C:17:DA:H2'	3:C:18:DT:C7	2.29	0.63
2:B:45:PHE:O	2:B:49:ILE:HG13	1.98	0.63
2:B:88:LEU:HD21	2:B:93:PHE:HB2	1.81	0.63
1:A:222:GLN:HE22	1:A:256:ILE:HG23	1.64	0.63
3:C:17:DA:H2'	3:C:18:DT:H72	1.80	0.62
1:A:274:ILE:HG21	1:A:306:ASP:HB3	1.81	0.62
1:A:313:PHE:CZ	1:A:342:ALA:HA	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:DG:H2'	3:C:5:DG:C8	2.34	0.62
1:A:148:TYR:O	1:A:152:ARG:NH1	2.32	0.62
2:B:354:LYS:H	2:B:354:LYS:HD2	1.63	0.62
3:C:15:DG:N2	3:C:16:DT:C2	2.67	0.62
1:A:404:PRO:O	2:B:416:TYR:OH	2.05	0.62
1:A:11:SER:O	1:A:272:GLY:N	2.31	0.62
2:B:177:PRO:HA	2:B:334:VAL:HG12	1.82	0.62
3:C:18:DT:H3	4:D:3:DA:N6	1.97	0.61
1:A:122:ASN:O	1:A:126:ILE:N	2.25	0.61
2:B:49:ILE:HG22	2:B:53:ILE:HD11	1.82	0.61
1:A:253:ALA:O	1:A:257:SER:OG	2.17	0.61
1:A:287:LYS:N	1:A:328:TYR:OH	2.33	0.61
1:A:329:HIS:HE1	1:A:364:ARG:O	1.82	0.61
3:C:6:DT:H2''	3:C:7:DA:C8	2.35	0.61
1:A:95:GLU:HG2	1:A:96:ILE:N	2.14	0.61
1:A:336:LYS:O	1:A:340:THR:OG1	2.18	0.61
2:B:249:GLY:HA2	2:B:258:ASN:HD22	1.65	0.61
1:A:481:ARG:HH12	4:D:19:DC:P	2.24	0.61
2:B:220:GLU:N	2:B:220:GLU:OE2	2.34	0.60
2:B:195:PRO:O	2:B:209:ARG:NH1	2.35	0.60
2:B:230:THR:C	2:B:232:THR:H	2.05	0.60
1:A:417:LYS:HB3	1:A:444:GLU:HG3	1.82	0.60
2:B:88:LEU:HG	2:B:90:ASP:HB3	1.82	0.60
2:B:241:ILE:HG22	2:B:246:ILE:HD11	1.82	0.60
2:B:109:ASN:O	2:B:113:VAL:HG23	2.02	0.60
2:B:18:THR:O	2:B:22:SER:OG	2.17	0.60
2:B:328:LYS:HD3	2:B:330:TYR:O	2.02	0.60
2:B:326:ALA:O	2:B:336:MET:N	2.34	0.60
1:A:236:ASN:HB3	1:A:242:ILE:HG12	1.83	0.60
1:A:362:ARG:NH2	1:A:476:GLU:OE2	2.35	0.60
1:A:478:VAL:HA	1:A:481:ARG:HB3	1.84	0.60
2:B:321:PHE:HD1	2:B:380:PHE:CD2	2.20	0.59
2:B:294:TRP:HZ2	2:B:350:LEU:CD1	2.13	0.59
2:B:358:HIS:NE2	4:D:14:DT:OP2	2.23	0.59
1:A:9:GLU:CD	1:A:10:PRO:HD2	2.22	0.59
1:A:425:PHE:CZ	1:A:430:GLN:HA	2.37	0.59
2:B:200:VAL:O	2:B:203:LEU:HB2	2.01	0.59
1:A:416:LYS:O	1:A:445:ILE:HG13	2.02	0.59
2:B:276:ARG:NH2	2:B:386:ASP:OD2	2.35	0.59
1:A:336:LYS:HA	1:A:376:VAL:HG21	1.85	0.59
2:B:175:TRP:HB2	2:B:408:LEU:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:TRP:O	2:B:372:LYS:N	2.35	0.59
2:B:190:TYR:HB3	2:B:194:LEU:HB3	1.85	0.59
1:A:369:GLU:O	1:A:372:ALA:HB3	2.03	0.58
1:A:57:LEU:HD21	1:A:86:TRP:CE2	2.39	0.58
1:A:50:LEU:HD11	1:A:91:ILE:HG21	1.84	0.58
1:A:271:LEU:HG	1:A:465:LEU:HD21	1.84	0.58
2:B:346:ASP:OD1	2:B:349:ASN:HB2	2.04	0.58
1:A:50:LEU:HD23	1:A:93:PHE:CD2	2.39	0.58
2:B:167:LYS:O	2:B:414:MET:N	2.31	0.58
4:D:4:DT:H6	4:D:4:DT:H5''	1.66	0.58
1:A:50:LEU:HD12	1:A:54:LYS:HE3	1.86	0.58
1:A:274:ILE:HG21	1:A:306:ASP:CB	2.34	0.58
1:A:416:LYS:HZ2	1:A:449:GLU:HG3	1.69	0.58
1:A:160:GLU:N	1:A:160:GLU:OE2	2.37	0.57
1:A:416:LYS:NZ	1:A:449:GLU:HG3	2.18	0.57
2:B:188:HIS:O	2:B:214:LEU:N	2.36	0.57
1:A:12:ILE:HG13	1:A:14:PHE:CZ	2.40	0.57
2:B:173:SER:OG	2:B:174:ASN:N	2.37	0.57
2:B:255:PHE:CD2	2:B:256:ILE:HG23	2.39	0.57
2:B:10:ALA:HB3	2:B:14:ASP:OD2	2.03	0.57
1:A:503:PHE:O	1:A:506:TYR:N	2.38	0.57
4:D:8:DA:H2''	4:D:9:DC:O5'	2.04	0.57
1:A:64:ILE:HD11	1:A:253:ALA:HB2	1.86	0.57
2:B:265:ILE:HG22	2:B:269:ILE:HD11	1.86	0.57
2:B:282:VAL:CG1	2:B:295:ILE:HG12	2.34	0.57
1:A:225:ARG:HE	1:A:227:SER:CB	2.18	0.57
2:B:190:TYR:HE2	2:B:227:LEU:HD11	1.70	0.57
2:B:344:THR:HG22	2:B:349:ASN:O	2.05	0.57
3:C:8:DG:C6	3:C:9:DT:C4	2.92	0.57
3:C:5:DG:C2	3:C:6:DT:C2	2.93	0.57
3:C:11:DG:H5'	3:C:12:DG:OP2	2.05	0.56
2:B:379:ALA:HA	2:B:382:ARG:HD2	1.85	0.56
2:B:320:HIS:HE2	2:B:344:THR:HG1	1.41	0.56
2:B:326:ALA:HB3	2:B:336:MET:HB2	1.87	0.56
2:B:344:THR:HB	2:B:346:ASP:O	2.05	0.56
4:D:11:DT:H2''	4:D:12:DA:O5'	2.06	0.56
1:A:165:LYS:HD3	1:A:165:LYS:N	2.20	0.56
1:A:321:TYR:HD2	1:A:322:ASN:H	1.53	0.56
2:B:305:PHE:CZ	2:B:383:PHE:HA	2.39	0.56
4:D:17:DC:H4'	4:D:18:DT:OP1	2.05	0.56
3:C:4:DG:N2	4:D:18:DT:C2	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLN:HG3	1:A:263:LYS:HE3	1.88	0.56
1:A:414:ASP:OD1	2:B:330:TYR:OH	2.23	0.56
2:B:203:LEU:O	2:B:205:PHE:N	2.39	0.55
1:A:304:PHE:HZ	1:A:503:PHE:CZ	2.23	0.55
2:B:150:SER:O	2:B:153:LEU:HB2	2.07	0.55
2:B:178:ILE:HD13	2:B:403:ILE:HG23	1.88	0.55
2:B:389:ASN:N	2:B:389:ASN:OD1	2.40	0.55
1:A:425:PHE:HA	1:A:432:THR:HA	1.89	0.55
2:B:2:ARG:HH11	2:B:2:ARG:N	2.02	0.55
3:C:15:DG:C2	4:D:7:DA:C2	2.95	0.55
1:A:225:ARG:HH21	1:A:227:SER:HG	1.53	0.55
1:A:347:LYS:HD2	1:A:353:TYR:CE1	2.42	0.54
2:B:206:PRO:HB2	2:B:268:LEU:HD23	1.88	0.54
1:A:58:ASP:OD1	1:A:58:ASP:N	2.39	0.54
2:B:112:ILE:HA	2:B:115:LEU:HD12	1.89	0.54
2:B:17:PHE:CZ	2:B:21:LEU:HB2	2.43	0.54
1:A:363:THR:O	1:A:387:THR:OG1	2.23	0.54
1:A:142:ILE:O	1:A:144:PRO:HD3	2.08	0.53
1:A:288:ILE:HD13	1:A:491:THR:HG23	1.90	0.53
1:A:391:SER:O	1:A:393:PRO:HD3	2.09	0.53
1:A:423:LEU:HG	1:A:434:SER:HB2	1.91	0.53
1:A:235:LYS:HA	1:A:241:PRO:HA	1.90	0.53
1:A:279:CYS:HB3	1:A:357:VAL:HG22	1.89	0.53
1:A:449:GLU:HG2	1:A:450:ALA:N	2.23	0.53
2:B:88:LEU:HD13	2:B:93:PHE:CD2	2.41	0.53
1:A:225:ARG:CZ	1:A:227:SER:OG	2.57	0.53
3:C:17:DA:C6	4:D:3:DA:N6	2.76	0.53
1:A:206:PHE:CE1	1:A:210:LEU:HD12	2.44	0.53
2:B:27:GLY:HA3	2:B:150:SER:HB2	1.91	0.52
1:A:24:ARG:HB2	1:A:73:PRO:HG2	1.92	0.52
2:B:45:PHE:O	2:B:48:THR:OG1	2.25	0.52
3:C:1:DT:H2''	3:C:2:DG:H5'	1.91	0.52
1:A:430:GLN:HE21	2:B:162:LYS:CB	2.21	0.52
2:B:59:LYS:NZ	2:B:140:VAL:HG22	2.24	0.52
4:D:20:DA:N3	4:D:20:DA:H2'	2.23	0.52
2:B:256:ILE:HG13	2:B:256:ILE:O	2.08	0.52
1:A:27:LEU:O	1:A:31:GLY:N	2.42	0.52
1:A:107:ASN:HD21	1:A:112:LYS:HD3	1.75	0.52
1:A:141:VAL:HB	1:A:223:ILE:HG12	1.92	0.52
2:B:321:PHE:HD1	2:B:380:PHE:HD2	1.56	0.52
1:A:398:LYS:HA	2:B:171:TYR:HD1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:CYS:HB3	2:B:37:LEU:CD2	2.38	0.52
2:B:206:PRO:HB2	2:B:268:LEU:CD2	2.39	0.52
1:A:50:LEU:HD21	1:A:93:PHE:CD2	2.45	0.52
1:A:93:PHE:CE2	1:A:95:GLU:HA	2.44	0.52
2:B:69:ASN:OD1	2:B:112:ILE:HD11	2.10	0.52
2:B:70:LYS:NZ	2:B:107:ASP:OD2	2.43	0.52
2:B:408:LEU:HD12	2:B:408:LEU:H	1.74	0.52
3:C:10:DA:N6	4:D:10:DC:N4	2.57	0.52
3:C:18:DT:H3	4:D:3:DA:H61	1.57	0.52
1:A:27:LEU:HD21	1:A:268:PRO:HB3	1.92	0.52
1:A:50:LEU:HD23	1:A:93:PHE:CE2	2.45	0.52
1:A:14:PHE:CE2	1:A:26:GLY:HA3	2.45	0.51
1:A:458:ASP:O	1:A:461:ALA:HB3	2.10	0.51
1:A:262:TYR:HE1	1:A:507:ILE:HD11	1.75	0.51
1:A:329:HIS:CG	1:A:366:ASN:HD22	2.28	0.51
1:A:405:ILE:HG22	2:B:171:TYR:CE1	2.45	0.51
1:A:66:ASN:N	1:A:66:ASN:HD22	2.06	0.51
1:A:351:LYS:N	1:A:351:LYS:HD2	2.26	0.51
1:A:406:MET:HB3	2:B:416:TYR:CD2	2.46	0.51
1:A:29:LEU:HB3	1:A:30:PHE:CD1	2.46	0.51
4:D:13:DC:H2"	4:D:14:DT:OP2	2.10	0.51
2:B:44:ASP:OD2	2:B:48:THR:HG23	2.11	0.51
2:B:193:ARG:O	2:B:195:PRO:HD3	2.11	0.51
1:A:40:LYS:HB3	1:A:136:VAL:HA	1.91	0.51
2:B:297:LYS:HE3	2:B:318:TYR:CE1	2.47	0.50
1:A:52:ILE:HG22	1:A:229:LEU:HB2	1.93	0.50
1:A:329:HIS:CG	1:A:366:ASN:ND2	2.79	0.50
2:B:354:LYS:H	2:B:354:LYS:CD	2.19	0.50
2:B:209:ARG:HB3	2:B:209:ARG:NH2	2.26	0.50
3:C:17:DA:C2	4:D:5:DA:N1	2.79	0.50
2:B:158:PHE:CD1	2:B:158:PHE:N	2.79	0.50
2:B:296:GLU:HB3	2:B:348:ILE:HG22	1.92	0.50
2:B:350:LEU:HD13	2:B:350:LEU:N	2.26	0.50
1:A:298:CYS:SG	1:A:490:LEU:HB3	2.51	0.50
2:B:66:THR:N	2:B:103:LEU:HD11	2.25	0.50
2:B:213:TYR:N	2:B:213:TYR:CD2	2.79	0.50
2:B:304:LYS:HE2	2:B:309:LYS:HB2	1.94	0.50
2:B:35:ASP:N	2:B:35:ASP:OD1	2.44	0.50
2:B:263:ARG:O	2:B:267:GLN:OE1	2.30	0.50
1:A:210:LEU:HD23	1:A:214:LEU:HD12	1.94	0.50
1:A:278:VAL:HG11	1:A:280:TYR:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:PHE:CD2	1:A:308:GLY:HA2	2.47	0.50
1:A:304:PHE:HD2	1:A:308:GLY:HA2	1.76	0.50
1:A:337:ALA:O	1:A:341:GLN:HB2	2.12	0.50
1:A:90:ASN:O	1:A:90:ASN:ND2	2.44	0.50
1:A:398:LYS:HE2	1:A:403:PHE:O	2.12	0.50
2:B:196:LYS:HA	2:B:209:ARG:NH1	2.27	0.50
2:B:383:PHE:CD1	2:B:384:LEU:HD23	2.47	0.49
1:A:368:GLU:OE2	1:A:369:GLU:N	2.45	0.49
1:A:407:ARG:NH1	1:A:422:THR:O	2.40	0.49
1:A:105:LEU:O	1:A:113:ARG:HD3	2.13	0.49
1:A:429:LEU:HD11	1:A:472:TYR:HB2	1.93	0.49
2:B:22:SER:HB3	2:B:32:VAL:HG11	1.94	0.49
1:A:30:PHE:HZ	2:B:151:ASN:HB3	1.77	0.49
1:A:133:GLU:OE1	1:A:133:GLU:N	2.40	0.49
2:B:285:TYR:HB3	2:B:292:ALA:HB3	1.93	0.49
2:B:285:TYR:N	2:B:292:ALA:O	2.44	0.49
1:A:389:THR:CG2	1:A:442:PHE:HB3	2.38	0.49
1:A:297:ALA:O	1:A:320:TRP:CD1	2.66	0.48
1:A:481:ARG:NH2	4:D:19:DC:OP2	2.42	0.48
2:B:128:LEU:O	2:B:132:LEU:HG	2.13	0.48
2:B:5:ILE:N	2:B:31:GLU:O	2.45	0.48
2:B:165:ILE:O	2:B:167:LYS:N	2.46	0.48
4:D:17:DC:H2''	4:D:18:DT:C5'	2.39	0.48
1:A:42:GLY:HA3	1:A:136:VAL:HG11	1.95	0.48
1:A:109:SER:O	1:A:113:ARG:HB3	2.13	0.48
3:C:16:DT:H3	4:D:5:DA:H61	1.61	0.48
4:D:5:DA:H2''	4:D:6:DC:O5'	2.13	0.48
1:A:210:LEU:HD13	1:A:223:ILE:HD11	1.95	0.48
2:B:7:ILE:HG21	2:B:18:THR:HG22	1.96	0.48
1:A:127:THR:O	1:A:131:ASN:HB2	2.14	0.48
1:A:304:PHE:CE1	1:A:479:THR:HA	2.48	0.48
4:D:9:DC:H2''	4:D:10:DC:H5'	1.96	0.48
1:A:157:LEU:HG	1:A:161:LEU:HD12	1.95	0.48
1:A:158:PRO:HD2	1:A:161:LEU:HD12	1.96	0.48
1:A:349:GLN:HB3	1:A:350:ASN:ND2	2.29	0.48
1:A:404:PRO:HD2	1:A:425:PHE:HB2	1.94	0.48
1:A:78:PHE:CE2	1:A:86:TRP:HE3	2.31	0.48
1:A:132:ASP:HB3	1:A:134:GLU:O	2.14	0.48
2:B:26:ILE:HG21	2:B:153:LEU:CD2	2.44	0.48
1:A:300:ALA:HB2	1:A:490:LEU:HD21	1.96	0.48
1:A:339:LEU:HD22	1:A:339:LEU:HA	1.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:SER:HB2	2:B:60:PHE:CZ	2.49	0.47
2:B:129:GLN:O	2:B:133:ASP:HB2	2.13	0.47
2:B:277:MET:HG3	2:B:293:TYR:CE2	2.48	0.47
1:A:55:SER:O	1:A:59:LYS:HB2	2.14	0.47
1:A:33:LEU:HB2	1:A:269:TRP:HA	1.96	0.47
1:A:393:PRO:HB2	2:B:175:TRP:HZ2	1.79	0.47
2:B:96:PRO:O	2:B:118:ILE:HG22	2.15	0.47
2:B:175:TRP:HB2	2:B:408:LEU:HD11	1.97	0.47
2:B:178:ILE:H	2:B:178:ILE:HG12	1.37	0.47
1:A:57:LEU:HB2	1:A:88:SER:HB3	1.97	0.47
1:A:295:GLN:HG2	1:A:321:TYR:O	2.15	0.47
1:A:421:TRP:NE1	1:A:440:PRO:CD	2.77	0.47
1:A:504:LYS:HA	1:A:507:ILE:CD1	2.41	0.47
2:B:210:TYR:CE2	2:B:256:ILE:HG21	2.50	0.47
2:B:324:SER:O	2:B:337:VAL:HA	2.13	0.47
1:A:63:PRO:HG3	2:B:124:TRP:CE2	2.50	0.47
2:B:2:ARG:H	2:B:2:ARG:NH1	2.08	0.47
2:B:172:ASP:HB3	2:B:407:PRO:HG2	1.96	0.47
2:B:188:HIS:HA	2:B:238:SER:HG	1.78	0.47
1:A:138:VAL:HB	1:A:140:PHE:CZ	2.50	0.47
1:A:309:ASP:O	1:A:503:PHE:HB2	2.14	0.47
1:A:394:LEU:HG	2:B:175:TRP:CH2	2.50	0.47
4:D:10:DC:H1'	4:D:11:DT:H5'	1.97	0.47
1:A:110:THR:HA	1:A:113:ARG:HE	1.79	0.47
1:A:262:TYR:CE1	1:A:507:ILE:HD11	2.50	0.47
1:A:411:TYR:HB3	1:A:419:PHE:HB2	1.96	0.47
1:A:50:LEU:HD12	1:A:54:LYS:CE	2.45	0.47
1:A:148:TYR:CD2	4:D:20:DA:C2	3.03	0.47
1:A:217:HIS:H	1:A:217:HIS:CD2	2.33	0.47
2:B:300:LEU:HD22	2:B:305:PHE:HB2	1.97	0.47
2:B:391:ILE:O	2:B:402:LEU:HA	2.15	0.47
2:B:311:VAL:HG22	2:B:320:HIS:HB3	1.97	0.46
2:B:337:VAL:HG11	2:B:381:ILE:HD11	1.97	0.46
3:C:4:DG:C6	3:C:5:DG:C6	3.03	0.46
3:C:7:DA:C8	3:C:8:DG:N2	2.83	0.46
4:D:5:DA:C6	4:D:6:DC:C2	3.04	0.46
1:A:12:ILE:HG21	1:A:464:LYS:HB3	1.98	0.46
1:A:66:ASN:HD21	1:A:251:HIS:N	2.14	0.46
1:A:411:TYR:CE2	1:A:413:VAL:HG22	2.50	0.46
2:B:321:PHE:CD1	2:B:380:PHE:CD2	3.03	0.46
1:A:206:PHE:CZ	1:A:210:LEU:HD12	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ALA:O	1:A:376:VAL:HG23	2.16	0.46
1:A:23:PRO:O	1:A:27:LEU:HD12	2.15	0.46
1:A:304:PHE:CZ	1:A:503:PHE:CZ	3.03	0.46
1:A:393:PRO:CB	2:B:175:TRP:HZ2	2.28	0.46
1:A:397:TYR:CD1	1:A:437:VAL:HG11	2.51	0.46
1:A:78:PHE:CE2	1:A:86:TRP:CE3	3.04	0.46
1:A:89:GLN:HG3	1:A:90:ASN:N	2.30	0.46
2:B:262:GLN:O	2:B:329:LEU:HD21	2.15	0.46
2:B:383:PHE:HD1	2:B:384:LEU:HD23	1.80	0.46
2:B:343:PHE:HB2	2:B:357:GLN:NE2	2.27	0.46
2:B:413:LYS:O	2:B:414:MET:HB2	2.16	0.46
2:B:27:GLY:CA	2:B:150:SER:HB2	2.46	0.46
3:C:1:DT:C4	3:C:2:DG:C6	3.04	0.46
1:A:110:THR:O	1:A:114:THR:N	2.38	0.46
1:A:361:ALA:O	1:A:387:THR:HA	2.15	0.46
2:B:4:LYS:HA	2:B:31:GLU:HB3	1.97	0.46
1:A:143:VAL:HG21	4:D:20:DA:C8	2.51	0.46
1:A:144:PRO:HA	1:A:226:GLU:OE2	2.15	0.46
1:A:255:THR:HG23	1:A:469:ALA:HA	1.98	0.45
1:A:338:LEU:HD12	1:A:338:LEU:HA	1.86	0.45
2:B:62:ILE:HG23	2:B:96:PRO:HA	1.98	0.45
2:B:103:LEU:HD12	2:B:103:LEU:HA	1.69	0.45
2:B:293:TYR:O	2:B:322:GLY:HA2	2.16	0.45
2:B:390:ALA:HB1	2:B:403:ILE:O	2.16	0.45
1:A:397:TYR:CE2	2:B:377:LEU:HD22	2.50	0.45
3:C:3:DA:H2''	3:C:4:DG:O5'	2.16	0.45
2:B:118:ILE:HD11	2:B:131:LEU:N	2.31	0.45
2:B:295:ILE:H	2:B:295:ILE:HG13	1.57	0.45
1:A:324:GLU:HG3	4:D:8:DA:H3'	1.98	0.45
4:D:4:DT:H2''	4:D:5:DA:C8	2.52	0.45
1:A:149:LYS:HD2	1:A:149:LYS:HA	1.50	0.45
2:B:132:LEU:C	2:B:135:PHE:H	2.20	0.45
2:B:356:ILE:H	2:B:356:ILE:HG13	1.49	0.45
3:C:17:DA:H2'	3:C:18:DT:C5	2.52	0.45
2:B:286:GLN:HG3	2:B:291:PHE:CE1	2.52	0.45
2:B:296:GLU:CB	2:B:348:ILE:HG22	2.47	0.45
2:B:308:ILE:HG21	2:B:376:LYS:HA	1.98	0.45
4:D:3:DA:H2'	4:D:4:DT:O4'	2.17	0.45
2:B:265:ILE:HG22	2:B:269:ILE:CD1	2.46	0.45
2:B:344:THR:HG22	2:B:349:ASN:C	2.38	0.45
1:A:143:VAL:HG21	4:D:20:DA:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LEU:HD23	1:A:465:LEU:HD12	1.99	0.45
2:B:176:PHE:O	2:B:403:ILE:HG22	2.16	0.45
2:B:388:GLN:H	2:B:388:GLN:HG3	1.52	0.45
3:C:10:DA:H2'	3:C:11:DG:H1'	1.97	0.45
1:A:78:PHE:CE2	1:A:257:SER:HB3	2.52	0.45
1:A:420:LEU:HD12	1:A:421:TRP:H	1.82	0.44
2:B:219:TRP:HB3	2:B:221:TYR:CE2	2.52	0.44
3:C:16:DT:H2''	3:C:17:DA:C8	2.52	0.44
1:A:64:ILE:HG13	1:A:250:GLY:HA2	1.97	0.44
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.82	0.44
2:B:118:ILE:HG23	2:B:118:ILE:O	2.16	0.44
2:B:277:MET:HE3	2:B:384:LEU:HD13	1.99	0.44
2:B:320:HIS:CD2	2:B:320:HIS:N	2.85	0.44
3:C:10:DA:H2'	3:C:11:DG:C1'	2.47	0.44
1:A:64:ILE:HD11	1:A:253:ALA:CB	2.47	0.44
1:A:405:ILE:HG22	2:B:171:TYR:CZ	2.52	0.44
2:B:413:LYS:H	2:B:413:LYS:HG3	1.67	0.44
3:C:14:DT:H2''	3:C:15:DG:C8	2.52	0.44
1:A:15:ALA:HB2	1:A:32:PRO:O	2.18	0.44
1:A:148:TYR:HD2	4:D:20:DA:C2	2.35	0.44
1:A:332:PRO:O	1:A:336:LYS:HG3	2.17	0.44
2:B:67:ALA:O	2:B:71:ARG:HB2	2.17	0.44
2:B:270:ASN:HD22	2:B:270:ASN:H	1.65	0.44
1:A:329:HIS:ND1	1:A:369:GLU:OE2	2.50	0.44
2:B:203:LEU:HD12	2:B:223:PHE:CD1	2.47	0.44
2:B:282:VAL:HG21	2:B:293:TYR:HB3	1.98	0.44
1:A:498:THR:HB	1:A:501:LEU:HD11	2.00	0.44
2:B:65:SER:HA	2:B:100:ASP:HB2	1.99	0.44
2:B:225:HIS:C	2:B:225:HIS:CD2	2.91	0.44
1:A:56:TYR:O	1:A:59:LYS:N	2.51	0.44
1:A:80:ALA:HB1	2:B:20:TRP:CZ2	2.53	0.44
2:B:151:ASN:HA	2:B:154:TYR:HB3	1.98	0.44
4:D:11:DT:H6	4:D:11:DT:H2'	1.70	0.44
2:B:210:TYR:HE2	2:B:256:ILE:HG21	1.83	0.43
2:B:312:GLY:HA3	2:B:319:TRP:CE2	2.53	0.43
2:B:350:LEU:HD22	2:B:350:LEU:H	1.83	0.43
1:A:133:GLU:CG	1:A:134:GLU:H	2.30	0.43
1:A:493:SER:O	1:A:496:ILE:HD11	2.18	0.43
2:B:245:ASP:HB3	2:B:250:ARG:HB2	1.99	0.43
2:B:266:VAL:HG12	2:B:270:ASN:ND2	2.33	0.43
3:C:12:DG:N2	3:C:13:DT:O2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD13	1:A:17:GLY:HA2	2.01	0.43
1:A:333:LYS:HD2	1:A:333:LYS:HA	1.81	0.43
1:A:421:TRP:CE2	1:A:440:PRO:CB	2.99	0.43
2:B:60:PHE:HE1	2:B:62:ILE:HB	1.83	0.43
2:B:22:SER:H	2:B:22:SER:HG	1.48	0.43
4:D:14:DT:H6	4:D:14:DT:H2'	1.63	0.43
4:D:18:DT:H2''	4:D:19:DC:C6	2.53	0.43
1:A:146:GLU:H	1:A:146:GLU:HG2	1.41	0.43
1:A:222:GLN:HG3	1:A:263:LYS:CD	2.49	0.43
1:A:278:VAL:HG11	1:A:280:TYR:OH	2.18	0.43
1:A:304:PHE:CE1	1:A:478:VAL:HG13	2.53	0.43
2:B:23:LEU:HD11	2:B:158:PHE:CE2	2.53	0.43
1:A:280:TYR:O	1:A:303:MET:HA	2.19	0.43
1:A:286:LYS:HD2	1:A:487:GLY:HA3	2.00	0.43
1:A:307:ASN:OD1	1:A:308:GLY:N	2.52	0.43
1:A:397:TYR:HB3	2:B:374:ARG:HB2	2.01	0.43
2:B:300:LEU:HB3	2:B:304:LYS:O	2.19	0.43
1:A:218:THR:O	1:A:219:ILE:HG13	2.19	0.43
3:C:15:DG:N2	4:D:7:DA:C2	2.86	0.43
1:A:22:ASP:HB3	1:A:25:ASP:HB2	2.01	0.43
2:B:158:PHE:N	2:B:158:PHE:HD1	2.17	0.43
2:B:175:TRP:O	2:B:408:LEU:HD12	2.17	0.43
1:A:206:PHE:CD1	1:A:206:PHE:C	2.92	0.43
1:A:307:ASN:O	1:A:467:TYR:OH	2.37	0.43
1:A:321:TYR:HD2	1:A:322:ASN:N	2.16	0.43
1:A:396:LEU:CB	1:A:405:ILE:HD13	2.49	0.43
1:A:501:LEU:HD13	1:A:506:TYR:HE2	1.84	0.43
2:B:8:SER:HA	2:B:77:GLU:OE1	2.19	0.43
2:B:247:LEU:HD12	2:B:248:SER:N	2.34	0.43
2:B:344:THR:HA	2:B:351:ILE:HG12	2.01	0.43
4:D:7:DA:C2'	4:D:8:DA:H5''	2.49	0.43
1:A:31:GLY:HA2	1:A:81:VAL:O	2.19	0.42
1:A:78:PHE:CD2	1:A:86:TRP:HE3	2.36	0.42
1:A:318:GLY:HA3	1:A:320:TRP:CE2	2.53	0.42
1:A:422:THR:HG22	1:A:460:LEU:HD12	2.00	0.42
2:B:127:GLY:HA2	2:B:130:ASP:HB2	2.01	0.42
2:B:321:PHE:CD1	2:B:380:PHE:HD2	2.35	0.42
2:B:191:ASP:H	2:B:194:LEU:HD23	1.84	0.42
2:B:393:LEU:HD11	2:B:403:ILE:CD1	2.49	0.42
2:B:69:ASN:O	2:B:75:LEU:HD21	2.19	0.42
2:B:369:TRP:HA	2:B:369:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:TYR:CD2	1:A:322:ASN:N	2.87	0.42
2:B:21:LEU:HD12	2:B:21:LEU:HA	1.79	0.42
2:B:213:TYR:N	2:B:213:TYR:HD2	2.17	0.42
1:A:71:THR:HG22	1:A:431:SER:HB2	2.01	0.42
1:A:97:THR:OG1	1:A:100:GLU:HG3	2.20	0.42
1:A:211:LYS:HD3	1:A:507:ILE:O	2.20	0.42
1:A:485:LYS:HE3	4:D:19:DC:H5'	2.01	0.42
2:B:371:ASP:OD1	2:B:372:LYS:N	2.52	0.42
1:A:468:ASN:OD1	1:A:507:ILE:HG21	2.19	0.42
2:B:241:ILE:CG2	2:B:246:ILE:HD11	2.47	0.42
2:B:248:SER:HB3	2:B:250:ARG:HG2	2.01	0.42
1:A:219:ILE:HA	1:A:220:PRO:HD3	1.90	0.42
3:C:17:DA:H2'	3:C:18:DT:C6	2.54	0.42
1:A:133:GLU:HG2	1:A:134:GLU:N	2.34	0.42
1:A:297:ALA:HB1	1:A:328:TYR:HE1	1.84	0.42
2:B:17:PHE:CD1	2:B:17:PHE:C	2.90	0.42
2:B:126:LYS:O	2:B:129:GLN:HB3	2.20	0.42
3:C:17:DA:C2	4:D:5:DA:C2	3.08	0.42
1:A:32:PRO:HD3	1:A:82:PHE:HA	2.02	0.42
1:A:122:ASN:HD21	1:A:213:ARG:HB3	1.85	0.42
1:A:332:PRO:HD3	1:A:368:GLU:OE1	2.20	0.42
2:B:200:VAL:HG21	2:B:207:ALA:HB3	2.02	0.42
2:B:393:LEU:HD11	2:B:403:ILE:HD11	2.01	0.42
1:A:425:PHE:HZ	1:A:430:GLN:HA	1.83	0.42
1:A:10:PRO:HG3	1:A:461:ALA:HA	2.01	0.41
2:B:258:ASN:O	2:B:261:CYS:N	2.53	0.41
1:A:9:GLU:HG2	1:A:21:THR:HG21	2.01	0.41
1:A:140:PHE:HA	1:A:222:GLN:O	2.20	0.41
1:A:207:HIS:CD2	1:A:208:ASP:N	2.87	0.41
1:A:212:ALA:HB1	1:A:493:SER:HB2	2.02	0.41
2:B:118:ILE:CG2	2:B:118:ILE:O	2.68	0.41
2:B:172:ASP:HB3	2:B:407:PRO:CG	2.50	0.41
1:A:406:MET:HA	1:A:425:PHE:O	2.20	0.41
2:B:255:PHE:CE2	2:B:256:ILE:HG23	2.55	0.41
2:B:323:ILE:HD12	2:B:337:VAL:HG13	2.02	0.41
3:C:12:DG:C2	3:C:13:DT:C2	3.08	0.41
1:A:71:THR:O	1:A:429:LEU:HD22	2.20	0.41
2:B:320:HIS:CD2	2:B:344:THR:OG1	2.73	0.41
1:A:85:LYS:HB2	1:A:87:GLU:HG3	2.03	0.41
1:A:121:PHE:O	1:A:125:ILE:HG13	2.20	0.41
1:A:319:PRO:HD2	1:A:320:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:HD12	1:A:421:TRP:N	2.36	0.41
2:B:152:LEU:O	2:B:156:GLN:HB2	2.20	0.41
3:C:9:DT:H2''	3:C:10:DA:O4'	2.19	0.41
4:D:18:DT:H2''	4:D:19:DC:C5	2.55	0.41
2:B:311:VAL:HG22	2:B:320:HIS:CB	2.51	0.41
1:A:14:PHE:CZ	1:A:23:PRO:HA	2.56	0.41
1:A:358:PHE:HA	1:A:384:VAL:O	2.21	0.41
2:B:61:LEU:HD22	2:B:95:ILE:HB	2.03	0.41
2:B:288:SER:OG	4:D:13:DC:H5''	2.20	0.41
2:B:330:TYR:CG	2:B:331:PRO:HA	2.55	0.41
3:C:16:DT:H2''	3:C:17:DA:H8	1.86	0.41
3:C:17:DA:C2'	3:C:18:DT:C6	3.04	0.41
1:A:304:PHE:CZ	1:A:478:VAL:HG22	2.55	0.41
1:A:392:LYS:N	1:A:393:PRO:HD3	2.34	0.41
1:A:464:LYS:NZ	1:A:473:ALA:HB2	2.36	0.41
2:B:196:LYS:HD3	4:D:5:DA:H3'	2.03	0.41
2:B:230:THR:C	2:B:232:THR:N	2.72	0.41
3:C:5:DG:N2	3:C:6:DT:O2	2.54	0.41
3:C:15:DG:C2	3:C:16:DT:C2	3.09	0.41
4:D:10:DC:H6	4:D:10:DC:H2'	1.76	0.41
1:A:30:PHE:CZ	2:B:151:ASN:HB3	2.54	0.41
1:A:148:TYR:HD2	4:D:20:DA:C4	2.39	0.41
2:B:153:LEU:N	2:B:153:LEU:CD1	2.83	0.41
2:B:341:ILE:HG13	2:B:361:ARG:NE	2.36	0.41
3:C:11:DG:H3'	3:C:12:DG:C8	2.56	0.41
1:A:52:ILE:O	1:A:55:SER:HB2	2.21	0.40
1:A:141:VAL:HG11	1:A:210:LEU:CD1	2.51	0.40
1:A:224:LEU:HA	4:D:21:DT:OP2	2.20	0.40
2:B:170:THR:HA	2:B:410:PHE:O	2.21	0.40
2:B:203:LEU:C	2:B:205:PHE:H	2.24	0.40
2:B:280:LYS:HD2	2:B:280:LYS:HA	1.85	0.40
1:A:10:PRO:HD3	1:A:460:LEU:HD23	2.03	0.40
1:A:77:GLY:O	1:A:78:PHE:C	2.59	0.40
1:A:137:ASP:O	1:A:220:PRO:HG2	2.22	0.40
1:A:501:LEU:HB2	1:A:506:TYR:HE2	1.87	0.40
2:B:323:ILE:HD12	2:B:337:VAL:CG1	2.51	0.40
2:B:393:LEU:HD11	2:B:403:ILE:HG12	2.03	0.40
1:A:413:VAL:HG13	2:B:331:PRO:HG3	2.03	0.40
2:B:267:GLN:O	2:B:271:LYS:HB2	2.20	0.40
1:A:107:ASN:ND2	1:A:112:LYS:HD3	2.34	0.40
1:A:122:ASN:ND2	1:A:213:ARG:HG2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:HG2	1:A:134:GLU:H	1.86	0.40
2:B:13:GLU:H	2:B:13:GLU:HG2	1.34	0.40
2:B:14:ASP:O	2:B:18:THR:OG1	2.38	0.40
2:B:368:TRP:HE3	2:B:373:TRP:CD1	2.40	0.40
2:B:379:ALA:HA	2:B:382:ARG:HB2	2.03	0.40
1:A:329:HIS:CE1	1:A:364:ARG:O	2.69	0.40
2:B:41:LYS:HE2	2:B:41:LYS:HB3	1.94	0.40
2:B:335:LEU:HA	2:B:335:LEU:HD12	1.79	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	470/507 (93%)	443 (94%)	23 (5%)	4 (1%)	14	51
2	B	417/421 (99%)	377 (90%)	34 (8%)	6 (1%)	9	40
All	All	887/928 (96%)	820 (92%)	57 (6%)	10 (1%)	12	46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	166	GLU
2	B	414	MET
1	A	391	SER
2	B	195	PRO
1	A	393	PRO
2	B	189	ARG
2	B	49	ILE
1	A	445	ILE
1	A	323	PRO
2	B	331	PRO

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	414/446 (93%)	342 (83%)	72 (17%)	1	8
2	B	372/387 (96%)	293 (79%)	79 (21%)	1	5
All	All	786/833 (94%)	635 (81%)	151 (19%)	1	7

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	13	LEU
1	A	19	LYS
1	A	27	LEU
1	A	34	ASN
1	A	35	GLN
1	A	37	TYR
1	A	40	LYS
1	A	41	SER
1	A	48	LYS
1	A	50	LEU
1	A	58	ASP
1	A	65	TYR
1	A	68	ASN
1	A	74	MET
1	A	84	CYS
1	A	85	LYS
1	A	88	SER
1	A	97	THR
1	A	109	SER
1	A	111	HIS
1	A	113	ARG
1	A	123	ASP
1	A	131	ASN
1	A	132	ASP
1	A	134	GLU
1	A	137	ASP

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Mol	Chain	Res	Type
1	A	146	GLU
1	A	157	LEU
1	A	164	THR
1	A	165	LYS
1	A	205	GLN
1	A	209	GLN
1	A	213	ARG
1	A	215	LEU
1	A	217	HIS
1	A	225	ARG
1	A	228	THR
1	A	232	ARG
1	A	257	SER
1	A	267	LYS
1	A	275	ARG
1	A	281	LEU
1	A	286	LYS
1	A	289	GLU
1	A	293	ASN
1	A	321	TYR
1	A	325	LYS
1	A	333	LYS
1	A	339	LEU
1	A	340	THR
1	A	352	SER
1	A	362	ARG
1	A	364	ARG
1	A	367	ASP
1	A	368	GLU
1	A	370	TRP
1	A	375	GLU
1	A	379	LYS
1	A	394	LEU
1	A	399	THR
1	A	400	GLU
1	A	417	LYS
1	A	423	LEU
1	A	442	PHE
1	A	474	ASP
1	A	476	GLU
1	A	494	THR
1	A	497	LYS

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Mol	Chain	Res	Type
1	A	498	THR
1	A	503	PHE
1	A	504	LYS
2	B	1	MET
2	B	2	ARG
2	B	13	GLU
2	B	18	THR
2	B	19	ARG
2	B	22	SER
2	B	31	GLU
2	B	35	ASP
2	B	37	LEU
2	B	39	LEU
2	B	45	PHE
2	B	54	ARG
2	B	56	ASN
2	B	71	ARG
2	B	76	LYS
2	B	78	LEU
2	B	83	LYS
2	B	87	HIS
2	B	88	LEU
2	B	103	LEU
2	B	104	SER
2	B	106	ASP
2	B	107	ASP
2	B	110	ILE
2	B	128	LEU
2	B	133	ASP
2	B	138	GLN
2	B	153	LEU
2	B	159	LEU
2	B	169	GLU
2	B	178	ILE
2	B	186	ARG
2	B	190	TYR
2	B	192	TRP
2	B	194	LEU
2	B	196	LYS
2	B	197	GLN
2	B	208	ILE
2	B	209	ARG

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Mol	Chain	Res	Type
2	B	213	TYR
2	B	214	LEU
2	B	221	TYR
2	B	224	ILE
2	B	225	HIS
2	B	226	GLN
2	B	238	SER
2	B	239	ILE
2	B	244	SER
2	B	248	SER
2	B	255	PHE
2	B	257	ARG
2	B	280	LYS
2	B	290	THR
2	B	296	GLU
2	B	297	LYS
2	B	302	LYS
2	B	307	LYS
2	B	316	ASN
2	B	338	SER
2	B	339	SER
2	B	344	THR
2	B	350	LEU
2	B	353	SER
2	B	354	LYS
2	B	356	ILE
2	B	360	SER
2	B	362	ARG
2	B	363	LYS
2	B	370	ASN
2	B	373	TRP
2	B	374	ARG
2	B	385	SER
2	B	386	ASP
2	B	389	ASN
2	B	393	LEU
2	B	403	ILE
2	B	406	LYS
2	B	408	LEU
2	B	415	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	90	ASN
1	A	122	ASN
1	A	163	GLN
1	A	217	HIS
1	A	222	GLN
1	A	350	ASN
1	A	366	ASN
1	A	468	ASN
2	B	138	GLN
2	B	156	GLN
2	B	197	GLN
2	B	225	HIS
2	B	270	ASN
2	B	316	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	474/507 (93%)	-0.06	10 (2%) 63 51	262, 296, 352, 428	0
2	B	419/421 (99%)	0.03	13 (3%) 51 40	271, 317, 384, 408	0
3	C	21/21 (100%)	0.13	0 100 100	303, 336, 380, 383	0
4	D	19/20 (95%)	0.64	2 (10%) 13 15	294, 347, 382, 392	0
All	All	933/969 (96%)	0.00	25 (2%) 56 44	262, 307, 380, 428	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	99	ILE	5.1
2	B	295	ILE	5.0
2	B	181	PHE	3.9
1	A	121	PHE	3.7
1	A	350	ASN	3.6
2	B	356	ILE	3.4
1	A	283	LEU	3.3
2	B	220	GLU	2.9
1	A	301	ALA	2.8
2	B	131	LEU	2.8
1	A	409	ASN	2.7
1	A	82	PHE	2.6
2	B	244	SER	2.5
1	A	305	LEU	2.5
2	B	217	PHE	2.5
4	D	10	DC	2.5
1	A	338	LEU	2.4
2	B	401	ILE	2.4
2	B	218	ALA	2.3
1	A	256	ILE	2.3
2	B	120	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	117	LEU	2.2
4	D	9	DC	2.1
2	B	37	LEU	2.1
2	B	49	ILE	2.1

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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	D	101	1/1	0.46	0.12	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.