



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2025 – 04:39 PM JST

PDB ID : 9L9X
Title : Structure of SPARTA in complex with guide DNA and a 20nt target DNA
Authors : Hu, R.; Guo, C.; Liu, X.; Chen, J.; Liu, L.
Deposited on : 2024-12-31
Resolution : 6.70 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

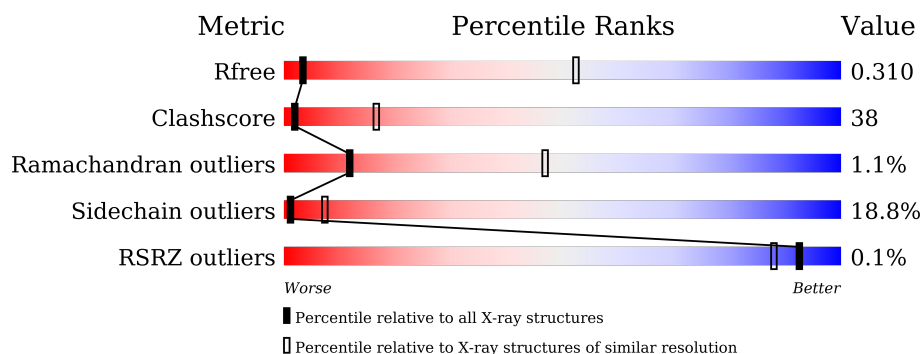
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.70 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	1101 (9.32-4.00)
Clashscore	180529	1141 (9.32-4.00)
Ramachandran outliers	177936	1010 (9.00-4.00)
Sidechain outliers	177891	1032 (9.00-3.96)
RSRZ outliers	164620	1096 (9.32-4.00)

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	
2	B	421	
3	C	21	
4	D	20	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8119 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(*TP*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	20	Total	C	N	O	P	0	0	0
			397	193	68	117	19			

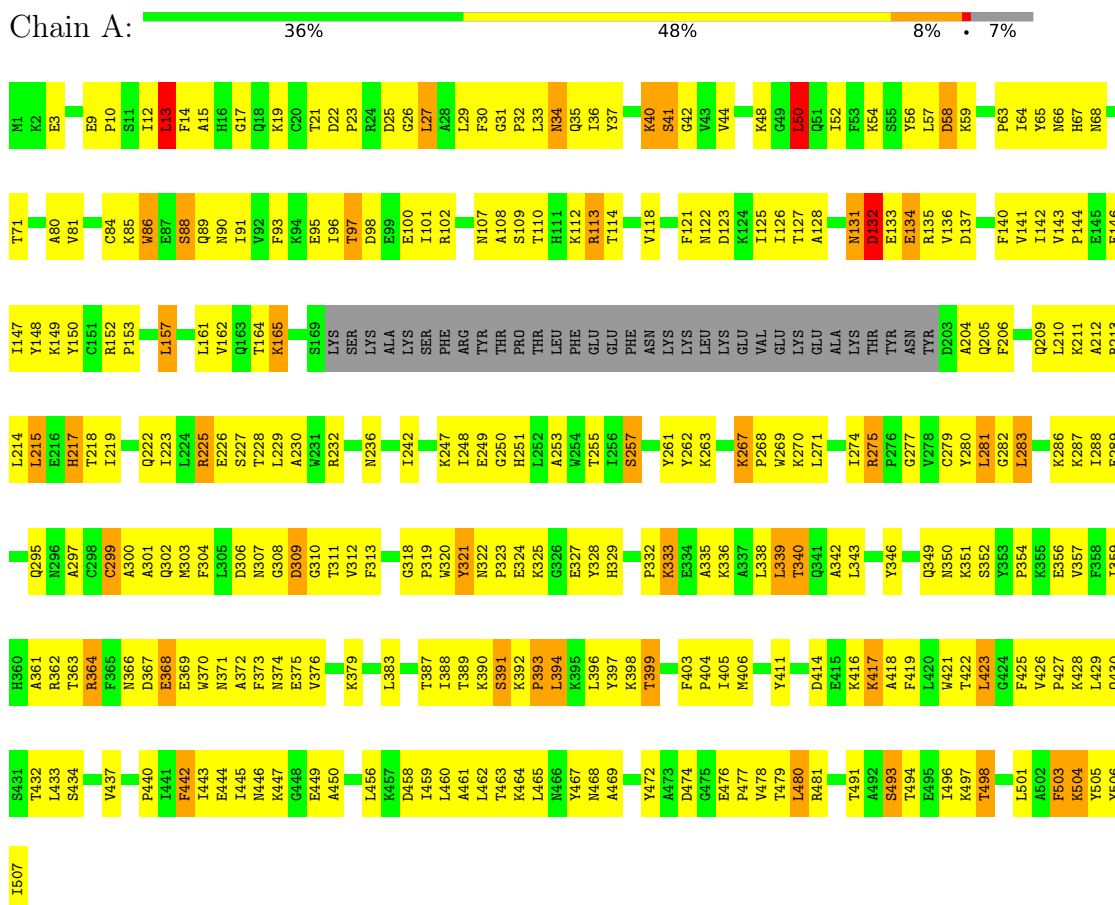
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

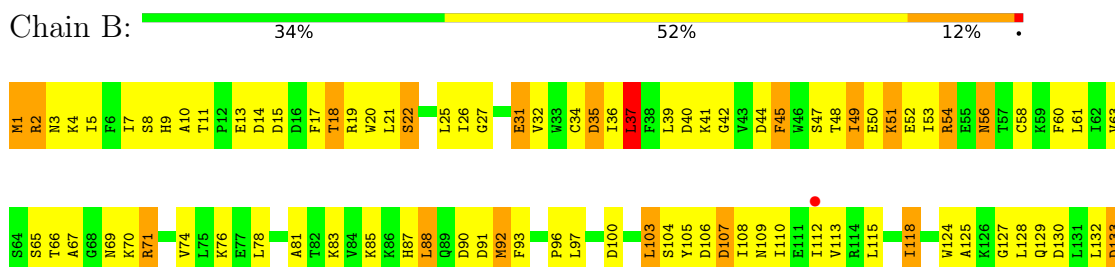
3 Residue-property plots [i](#)

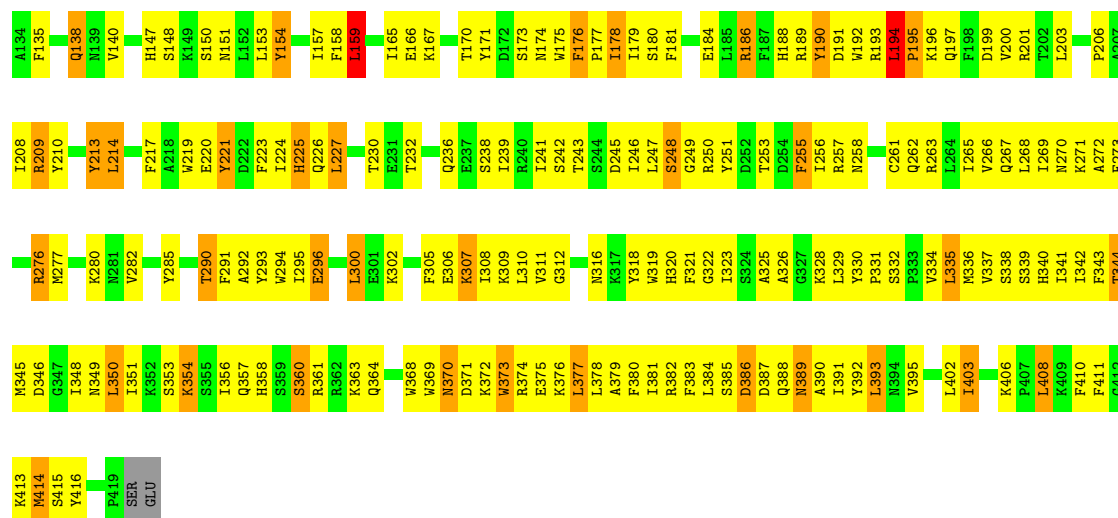
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Piwi domain-containing protein



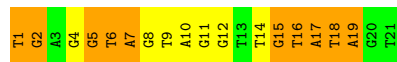
• Molecule 2: TIR domain-containing protein





- 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')

Chain C: 19% 33% 48%



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

Chain D: 80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.42Å 140.42Å 176.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.50 – 6.70 19.50 – 6.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.50-6.70) 94.8 (19.50-6.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 6.96Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.247 , 0.319 0.242 , 0.310	Depositor DCC
R_{free} test set	194 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	544.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 663.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8119	wwPDB-VP
Average B, all atoms (Å ²)	566.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	0.69	3/3923 (0.1%)	0.77	4/5313 (0.1%)
2	B	0.80	3/3539 (0.1%)	0.89	9/4780 (0.2%)
3	C	1.73	10/496 (2.0%)	1.39	6/765 (0.8%)
4	D	1.58	5/443 (1.1%)	1.33	3/679 (0.4%)
All	All	0.89	21/8401 (0.2%)	0.91	22/11537 (0.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	360	SER	CB-OG	-16.04	1.21	1.42
3	C	1	DT	C1'-N1	12.24	1.65	1.49
3	C	1	DT	OP3-P	-10.70	1.48	1.61
4	D	9	DC	C1'-N1	9.01	1.60	1.49
3	C	2	DG	N9-C8	8.13	1.43	1.37
2	B	176	PHE	CE2-CZ	-7.09	1.23	1.37
3	C	15	DG	C3'-O3'	7.09	1.53	1.44
4	D	18	DT	N1-C6	-6.75	1.33	1.38
3	C	16	DT	C3'-O3'	6.56	1.52	1.44
1	A	50	LEU	CG-CD2	6.08	1.74	1.51
1	A	86	TRP	CB-CG	-5.97	1.39	1.50
4	D	18	DT	C2-O2	5.71	1.27	1.22
3	C	7	DA	C3'-O3'	-5.68	1.36	1.44
4	D	18	DT	C5-C6	-5.67	1.30	1.34
3	C	19	DA	C3'-O3'	-5.59	1.36	1.44
2	B	42	GLY	CA-C	-5.50	1.43	1.51
3	C	6	DT	C1'-N1	5.25	1.56	1.49
3	C	5	DG	C3'-O3'	5.16	1.50	1.44
1	A	50	LEU	CB-CG	-5.06	1.37	1.52
4	D	10	DC	P-O5'	5.05	1.64	1.59
3	C	17	DA	N9-C4	5.05	1.40	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	276	ARG	NE-CZ-NH1	9.06	124.83	120.30
2	B	276	ARG	NE-CZ-NH2	-8.45	116.07	120.30
2	B	335	LEU	CA-CB-CG	-8.29	96.23	115.30
1	A	132	ASP	CB-CG-OD2	8.23	125.71	118.30
2	B	377	LEU	CA-CB-CG	7.19	131.83	115.30
2	B	176	PHE	CG-CD1-CE1	-6.91	113.20	120.80
1	A	283	LEU	CA-CB-CG	-6.10	101.28	115.30
3	C	16	DT	P-O3'-C3'	6.02	126.92	119.70
2	B	118	ILE	CG1-CB-CG2	-5.85	98.53	111.40
2	B	37	LEU	CA-CB-CG	5.76	128.54	115.30
1	A	309	ASP	CB-CG-OD1	5.75	123.48	118.30
3	C	18	DT	N3-C4-O4	5.49	123.19	119.90
1	A	13	LEU	CA-CB-CG	5.49	127.92	115.30
3	C	5	DG	O4'-C1'-N9	5.34	111.74	108.00
2	B	194	LEU	CA-CB-CG	5.28	127.44	115.30
4	D	18	DT	C5-C4-O4	-5.28	121.21	124.90
2	B	159	LEU	CA-CB-CG	5.23	127.33	115.30
3	C	2	DG	C4-C5-N7	5.21	112.88	110.80
3	C	16	DT	OP2-P-O3'	5.16	116.55	105.20
3	C	17	DA	O5'-P-OP1	-5.15	101.06	105.70
4	D	9	DC	O4'-C1'-N1	5.12	111.59	108.00
4	D	20	DA	OP2-P-O3'	5.07	116.35	105.20

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	3827	0	3844	288	0
2	B	3452	0	3416	261	1
3	C	442	0	240	43	1
4	D	397	0	228	48	0
5	D	1	0	0	0	0
All	All	8119	0	7728	599	1

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 38.

All (599) 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:463:THR:HB	1:A:474:ASP:O	1.42	1.15
1:A:390:LYS:CE	1:A:476:GLU:HG2	1.84	1.07
1:A:40:LYS:HG3	1:A:90:ASN:HD21	1.20	1.05
1:A:390:LYS:CE	1:A:476:GLU:CG	2.39	1.01
1:A:390:LYS:HE3	1:A:476:GLU:CG	1.92	1.00
1:A:463:THR:HA	1:A:474:ASP:HB3	1.43	0.98
1:A:463:THR:CA	1:A:474:ASP:HB3	1.93	0.98
2:B:184:GLU:O	2:B:186:ARG:NH2	1.97	0.97
3:C:1:DT:H2''	3:C:2:DG:H5'	1.45	0.95
1:A:390:LYS:HE2	1:A:476:GLU:HG2	1.50	0.93
1:A:302:GLN:NE2	1:A:479:THR:O	2.02	0.92
1:A:468:ASN:HD21	1:A:507:ILE:HD13	1.33	0.92
1:A:463:THR:O	1:A:474:ASP:CB	2.18	0.91
3:C:14:DT:H3	4:D:7:DA:H61	1.13	0.90
1:A:463:THR:CB	1:A:474:ASP:O	2.18	0.89
2:B:206:PRO:HG3	2:B:395:VAL:HG12	1.54	0.89
4:D:2:DT:H1'	4:D:3:DA:C8	2.07	0.89
1:A:52:ILE:HD12	1:A:226:GLU:HG2	1.54	0.88
4:D:2:DT:H1'	4:D:3:DA:H8	1.40	0.85
1:A:399:THR:OG1	2:B:170:THR:O	1.96	0.84
1:A:432:THR:OG1	1:A:434:SER:O	1.95	0.84
2:B:310:LEU:HD13	2:B:380:PHE:CD2	2.15	0.81
1:A:463:THR:O	1:A:474:ASP:HB2	1.80	0.81
2:B:305:PHE:CZ	2:B:383:PHE:HA	2.16	0.81
2:B:199:ASP:OD1	2:B:201:ARG:NH2	2.14	0.81
1:A:390:LYS:HE3	1:A:476:GLU:OE2	1.80	0.80
1:A:153:PRO:HG3	1:A:204:ALA:HB3	1.62	0.80
2:B:2:ARG:HH11	2:B:2:ARG:H	1.29	0.80
2:B:188:HIS:HA	2:B:238:SER:HG	1.45	0.79
3:C:19:DA:N6	4:D:2:DT:O4	2.15	0.79
2:B:188:HIS:HA	2:B:238:SER:OG	1.81	0.78
1:A:225:ARG:NE	1:A:227:SER:OG	2.15	0.78
1:A:389:THR:HG23	1:A:442:PHE:HB3	1.63	0.78
1:A:128:ALA:O	1:A:132:ASP:HB2	1.84	0.78
1:A:127:THR:O	1:A:131:ASN:HB2	1.84	0.78
3:C:17:DA:H2'	3:C:18:DT:C7	2.15	0.77
3:C:11:DG:N2	4:D:11:DT:O2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:VAL:HG12	2:B:295:ILE:HG12	1.66	0.76
2:B:312:GLY:HA3	2:B:319:TRP:CE2	2.20	0.76
2:B:249:GLY:HA2	2:B:258:ASN:HD22	1.50	0.76
1:A:268:PRO:HB2	1:A:269:TRP:CE3	2.21	0.76
1:A:9:GLU:OE1	1:A:464:LYS:NZ	2.19	0.76
2:B:65:SER:O	2:B:69:ASN:ND2	2.20	0.75
4:D:6:DC:H2''	4:D:7:DA:C8	2.21	0.75
2:B:294:TRP:HZ2	2:B:350:LEU:HD12	1.50	0.75
1:A:416:LYS:O	1:A:445:ILE:HG13	1.87	0.74
4:D:12:DA:H2''	4:D:13:DC:H5'	1.66	0.74
1:A:463:THR:HB	1:A:474:ASP:C	2.08	0.74
4:D:20:DA:H4'	4:D:21:DT:OP2	1.88	0.74
2:B:61:LEU:HB3	2:B:97:LEU:HD11	1.67	0.73
2:B:241:ILE:HG22	2:B:246:ILE:HD11	1.70	0.73
1:A:262:TYR:OH	1:A:309:ASP:OD1	2.03	0.73
1:A:327:GLU:OE2	1:A:329:HIS:NE2	2.22	0.73
1:A:468:ASN:HD21	1:A:507:ILE:CD1	2.00	0.72
1:A:143:VAL:HG13	1:A:147:ILE:HB	1.71	0.72
1:A:122:ASN:HD22	1:A:213:ARG:HG2	1.54	0.72
2:B:380:PHE:O	2:B:383:PHE:HB3	1.90	0.72
3:C:4:DG:H2'	3:C:5:DG:C8	2.25	0.72
1:A:122:ASN:O	1:A:126:ILE:N	2.17	0.71
1:A:59:LYS:NZ	1:A:249:GLU:OE1	2.18	0.71
1:A:421:TRP:CZ2	1:A:440:PRO:HG3	2.26	0.71
1:A:390:LYS:HE3	1:A:476:GLU:CD	2.11	0.71
1:A:398:LYS:HE2	1:A:403:PHE:O	1.90	0.71
1:A:40:LYS:HG3	1:A:90:ASN:ND2	2.02	0.71
1:A:503:PHE:O	1:A:506:TYR:N	2.22	0.71
2:B:294:TRP:CZ2	2:B:350:LEU:HD12	2.25	0.71
2:B:105:TYR:CE1	2:B:113:VAL:HG11	2.26	0.71
1:A:93:PHE:CZ	1:A:95:GLU:HA	2.26	0.71
2:B:294:TRP:HB3	2:B:342:ILE:HG13	1.71	0.71
2:B:147:HIS:O	2:B:150:SER:HB3	1.91	0.70
2:B:177:PRO:HA	2:B:334:VAL:HA	1.73	0.70
2:B:97:LEU:HA	2:B:118:ILE:HG22	1.73	0.70
2:B:343:PHE:HB2	2:B:357:GLN:HE21	1.57	0.70
2:B:109:ASN:O	2:B:113:VAL:HG23	1.91	0.69
4:D:17:DC:H2''	4:D:18:DT:H5''	1.73	0.69
2:B:97:LEU:HA	2:B:118:ILE:CG2	2.21	0.69
4:D:15:DA:H2''	4:D:16:DC:H5''	1.73	0.69
1:A:67:HIS:N	1:A:247:LYS:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:HD23	2:B:118:ILE:HG21	1.73	0.69
2:B:22:SER:HB3	2:B:32:VAL:HG11	1.73	0.69
2:B:358:HIS:NE2	4:D:14:DT:OP2	2.17	0.69
1:A:271:LEU:HG	1:A:465:LEU:HD21	1.73	0.69
1:A:421:TRP:CE2	1:A:440:PRO:HB3	2.28	0.69
1:A:421:TRP:CD2	1:A:440:PRO:HB3	2.28	0.68
1:A:390:LYS:CE	1:A:476:GLU:OE2	2.41	0.68
1:A:279:CYS:SG	1:A:281:LEU:HD22	2.34	0.68
1:A:141:VAL:HB	1:A:223:ILE:HG12	1.77	0.67
1:A:404:PRO:O	2:B:416:TYR:OH	2.02	0.67
2:B:220:GLU:N	2:B:220:GLU:OE2	2.27	0.67
1:A:463:THR:CG2	1:A:474:ASP:O	2.42	0.67
2:B:379:ALA:HA	2:B:382:ARG:HD2	1.76	0.66
3:C:18:DT:H3	4:D:3:DA:N6	1.93	0.66
1:A:463:THR:O	1:A:474:ASP:HB3	1.95	0.66
2:B:305:PHE:O	2:B:307:LYS:N	2.29	0.66
2:B:369:TRP:O	2:B:372:LYS:N	2.28	0.66
1:A:10:PRO:HG3	1:A:461:ALA:HA	1.78	0.66
2:B:167:LYS:O	2:B:414:MET:N	2.27	0.66
2:B:236:GLN:N	2:B:236:GLN:OE1	2.28	0.66
1:A:504:LYS:HA	1:A:507:ILE:HD12	1.77	0.65
1:A:133:GLU:OE1	1:A:133:GLU:N	2.28	0.65
2:B:379:ALA:O	2:B:383:PHE:N	2.29	0.65
1:A:390:LYS:HE3	1:A:476:GLU:HG3	1.75	0.65
1:A:44:VAL:HG21	1:A:125:ILE:HG12	1.77	0.65
1:A:50:LEU:CD2	1:A:93:PHE:CD2	2.80	0.65
2:B:108:ILE:HB	2:B:113:VAL:HG22	1.78	0.65
2:B:203:LEU:HD12	2:B:223:PHE:HD1	1.62	0.65
3:C:17:DA:H2'	3:C:18:DT:H72	1.76	0.65
1:A:108:ALA:HB2	1:A:162:VAL:HG11	1.77	0.65
2:B:325:ALA:HB1	2:B:335:LEU:HD11	1.79	0.65
2:B:326:ALA:HB3	2:B:336:MET:HB2	1.77	0.65
1:A:29:LEU:HB3	1:A:30:PHE:CE1	2.31	0.64
1:A:425:PHE:CZ	1:A:430:GLN:HA	2.32	0.64
2:B:2:ARG:HH11	2:B:2:ARG:N	1.96	0.64
2:B:11:THR:HG22	2:B:15:ASP:OD1	1.96	0.64
2:B:27:GLY:HA3	2:B:150:SER:HB2	1.79	0.64
1:A:397:TYR:CD1	1:A:437:VAL:HG11	2.32	0.64
1:A:222:GLN:HG3	1:A:263:LYS:HE3	1.80	0.64
1:A:299:CYS:SG	1:A:300:ALA:N	2.72	0.63
2:B:176:PHE:O	2:B:335:LEU:N	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LYS:NZ	2:B:107:ASP:OD2	2.32	0.63
3:C:15:DG:C2	4:D:7:DA:C2	2.87	0.62
2:B:96:PRO:O	2:B:118:ILE:HG22	1.99	0.62
1:A:282:GLY:O	1:A:301:ALA:HA	1.99	0.62
3:C:10:DA:N6	4:D:10:DC:N4	2.47	0.62
1:A:463:THR:C	1:A:474:ASP:HB3	2.20	0.62
2:B:4:LYS:NZ	2:B:52:GLU:OE1	2.28	0.62
2:B:88:LEU:HD21	2:B:93:PHE:HB2	1.82	0.62
1:A:14:PHE:CE2	1:A:26:GLY:HA3	2.34	0.62
2:B:177:PRO:HA	2:B:334:VAL:HG12	1.80	0.62
3:C:6:DT:H2''	3:C:7:DA:C8	2.35	0.61
1:A:36:ILE:HG23	1:A:261:TYR:OH	1.99	0.61
1:A:50:LEU:HD23	1:A:93:PHE:CD2	2.36	0.61
2:B:354:LYS:H	2:B:354:LYS:HD2	1.64	0.61
1:A:463:THR:O	1:A:474:ASP:N	2.33	0.61
1:A:14:PHE:CZ	1:A:23:PRO:HA	2.35	0.61
1:A:148:TYR:O	1:A:152:ARG:NH1	2.33	0.61
2:B:190:TYR:HB3	2:B:194:LEU:HB3	1.83	0.61
2:B:276:ARG:NH2	2:B:386:ASP:OD2	2.34	0.61
1:A:274:ILE:HG21	1:A:306:ASP:HB3	1.82	0.60
2:B:246:ILE:HG21	2:B:261:CYS:SG	2.41	0.60
1:A:212:ALA:HB1	1:A:493:SER:HB2	1.84	0.60
2:B:267:GLN:O	2:B:271:LYS:N	2.28	0.60
2:B:346:ASP:OD1	2:B:349:ASN:HB2	2.01	0.60
1:A:89:GLN:HG3	1:A:90:ASN:N	2.16	0.60
1:A:406:MET:HE3	1:A:427:PRO:HD3	1.84	0.60
2:B:81:ALA:O	2:B:85:LYS:N	2.35	0.60
1:A:304:PHE:HD2	1:A:308:GLY:HA2	1.67	0.59
1:A:391:SER:C	1:A:393:PRO:HD3	2.22	0.59
2:B:27:GLY:CA	2:B:150:SER:HB2	2.32	0.59
3:C:15:DG:N2	3:C:16:DT:C2	2.70	0.59
1:A:14:PHE:CZ	1:A:26:GLY:HA3	2.37	0.59
2:B:305:PHE:O	2:B:308:ILE:N	2.36	0.59
3:C:4:DG:C6	3:C:5:DG:C6	2.91	0.59
1:A:307:ASN:OD1	1:A:308:GLY:N	2.35	0.59
1:A:417:LYS:HB3	1:A:444:GLU:HG3	1.83	0.59
1:A:446:ASN:O	1:A:447:LYS:HD3	2.03	0.59
1:A:414:ASP:OD1	2:B:330:TYR:OH	2.19	0.59
2:B:49:ILE:HG22	2:B:53:ILE:HD11	1.85	0.59
2:B:296:GLU:HB3	2:B:348:ILE:HG22	1.83	0.59
1:A:336:LYS:HA	1:A:376:VAL:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:PRO:HB2	2:B:175:TRP:HZ2	1.66	0.58
1:A:427:PRO:O	1:A:430:GLN:HG2	2.02	0.58
1:A:463:THR:HB	1:A:474:ASP:CA	2.33	0.58
2:B:17:PHE:CZ	2:B:21:LEU:HB2	2.38	0.58
1:A:393:PRO:CB	2:B:175:TRP:HZ2	2.15	0.58
1:A:90:ASN:ND2	1:A:90:ASN:O	2.36	0.58
2:B:344:THR:HB	2:B:346:ASP:O	2.03	0.58
4:D:4:DT:H6	4:D:4:DT:H5''	1.67	0.58
1:A:66:ASN:N	1:A:66:ASN:HD22	2.00	0.58
1:A:107:ASN:HD21	1:A:112:LYS:HD3	1.67	0.58
2:B:285:TYR:N	2:B:292:ALA:O	2.33	0.58
1:A:64:ILE:HD11	1:A:253:ALA:HB2	1.85	0.57
2:B:190:TYR:HE2	2:B:227:LEU:HD11	1.69	0.57
2:B:217:PHE:HB2	2:B:395:VAL:HB	1.86	0.57
2:B:321:PHE:HD1	2:B:380:PHE:CD2	2.22	0.57
1:A:165:LYS:HD3	1:A:165:LYS:N	2.18	0.57
1:A:425:PHE:HA	1:A:432:THR:HA	1.85	0.57
1:A:287:LYS:N	1:A:328:TYR:OH	2.37	0.57
2:B:58:CYS:SG	2:B:140:VAL:HG13	2.44	0.57
2:B:255:PHE:CD2	2:B:256:ILE:HG23	2.38	0.57
2:B:209:ARG:HH21	2:B:209:ARG:HB3	1.70	0.57
1:A:253:ALA:O	1:A:257:SER:OG	2.16	0.57
2:B:328:LYS:HD3	2:B:330:TYR:O	2.03	0.57
2:B:393:LEU:HD11	2:B:403:ILE:CG1	2.34	0.57
2:B:300:LEU:HD22	2:B:305:PHE:HB2	1.87	0.57
1:A:57:LEU:HB2	1:A:88:SER:HB3	1.86	0.57
2:B:320:HIS:NE2	2:B:344:THR:OG1	2.38	0.57
3:C:14:DT:H2''	3:C:15:DG:C8	2.40	0.57
1:A:50:LEU:HD12	1:A:54:LYS:HE3	1.87	0.56
1:A:468:ASN:ND2	1:A:507:ILE:HD13	2.13	0.56
2:B:354:LYS:HA	2:B:357:GLN:HB2	1.87	0.56
1:A:397:TYR:HE2	2:B:174:ASN:HB3	1.71	0.56
2:B:10:ALA:HB3	2:B:14:ASP:OD2	2.05	0.56
2:B:195:PRO:O	2:B:209:ARG:NH1	2.37	0.56
1:A:329:HIS:HE1	1:A:364:ARG:O	1.88	0.56
1:A:418:ALA:HB3	1:A:456:LEU:HD21	1.88	0.56
2:B:206:PRO:HB2	2:B:268:LEU:CD2	2.36	0.56
2:B:341:ILE:HB	2:B:361:ARG:HD3	1.88	0.56
2:B:393:LEU:HD11	2:B:403:ILE:HG12	1.88	0.56
1:A:64:ILE:HG13	1:A:250:GLY:HA2	1.88	0.55
2:B:256:ILE:HG13	2:B:256:ILE:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:ND2	1:A:213:ARG:HG2	2.21	0.55
2:B:92:MET:HG2	2:B:138:GLN:NE2	2.21	0.55
1:A:275:ARG:NH1	1:A:458:ASP:OD2	2.40	0.55
2:B:241:ILE:CG2	2:B:246:ILE:HD11	2.36	0.55
1:A:52:ILE:HG22	1:A:229:LEU:HB2	1.89	0.55
1:A:222:GLN:HG3	1:A:263:LYS:CD	2.36	0.55
2:B:34:CYS:HB3	2:B:37:LEU:HD22	1.88	0.55
2:B:277:MET:HG3	2:B:293:TYR:CE2	2.41	0.55
3:C:17:DA:C6	4:D:3:DA:N6	2.74	0.55
1:A:14:PHE:CE1	1:A:23:PRO:HA	2.41	0.55
1:A:274:ILE:HG21	1:A:306:ASP:CB	2.36	0.55
2:B:243:THR:HA	2:B:246:ILE:HG12	1.88	0.55
1:A:97:THR:OG1	1:A:100:GLU:HG3	2.06	0.55
3:C:1:DT:C4	3:C:2:DG:C6	2.95	0.54
3:C:18:DT:H3	4:D:3:DA:H61	1.55	0.54
1:A:157:LEU:HG	1:A:161:LEU:HD12	1.90	0.54
1:A:426:VAL:O	1:A:430:GLN:N	2.41	0.54
2:B:14:ASP:O	2:B:18:THR:OG1	2.23	0.54
3:C:11:DG:H2'	3:C:12:DG:C5	2.42	0.54
1:A:318:GLY:HA3	1:A:320:TRP:CZ2	2.41	0.54
2:B:37:LEU:HA	2:B:157:ILE:HG21	1.90	0.54
1:A:283:LEU:HB2	1:A:361:ALA:HB2	1.87	0.54
1:A:332:PRO:O	1:A:336:LYS:HG3	2.07	0.54
1:A:107:ASN:ND2	1:A:112:LYS:HD3	2.23	0.54
4:D:8:DA:H2''	4:D:9:DC:O5'	2.07	0.54
1:A:206:PHE:CE1	1:A:210:LEU:HD12	2.43	0.54
2:B:180:SER:OG	2:B:402:LEU:HB2	2.08	0.54
2:B:193:ARG:O	2:B:195:PRO:HD3	2.08	0.54
4:D:20:DA:N3	4:D:20:DA:H2'	2.21	0.54
1:A:405:ILE:HG22	2:B:171:TYR:CZ	2.43	0.53
4:D:4:DT:H2''	4:D:5:DA:C8	2.43	0.53
1:A:222:GLN:HG3	1:A:263:LYS:CE	2.39	0.53
2:B:210:TYR:CE2	2:B:256:ILE:HG21	2.44	0.53
2:B:310:LEU:HD13	2:B:380:PHE:HD2	1.70	0.53
1:A:13:LEU:HD13	1:A:17:GLY:HA2	1.91	0.53
2:B:230:THR:C	2:B:232:THR:H	2.11	0.53
2:B:294:TRP:HZ2	2:B:350:LEU:CD1	2.19	0.53
1:A:41:SER:HB3	1:A:86:TRP:HE1	1.74	0.53
1:A:95:GLU:HG2	1:A:96:ILE:N	2.24	0.53
1:A:295:GLN:NE2	1:A:321:TYR:O	2.30	0.53
2:B:383:PHE:CD1	2:B:384:LEU:HD23	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HD23	1:A:93:PHE:CE2	2.44	0.53
1:A:304:PHE:CD2	1:A:308:GLY:HA2	2.43	0.53
4:D:9:DC:H2''	4:D:10:DC:H5'	1.91	0.53
1:A:303:MET:HE2	1:A:311:THR:HB	1.90	0.53
1:A:389:THR:CG2	1:A:442:PHE:HB3	2.34	0.53
2:B:290:THR:OG1	2:B:291:PHE:N	2.42	0.53
2:B:389:ASN:N	2:B:389:ASN:OD1	2.42	0.53
1:A:281:LEU:HB2	1:A:359:ILE:HG12	1.91	0.52
2:B:45:PHE:O	2:B:48:THR:OG1	2.26	0.52
2:B:312:GLY:HA3	2:B:319:TRP:NE1	2.24	0.52
1:A:361:ALA:O	1:A:387:THR:HA	2.09	0.52
2:B:92:MET:HG2	2:B:138:GLN:HE22	1.72	0.52
1:A:279:CYS:HB3	1:A:357:VAL:HG22	1.92	0.52
2:B:210:TYR:HE2	2:B:256:ILE:HG21	1.74	0.52
1:A:58:ASP:OD1	1:A:58:ASP:N	2.42	0.52
2:B:174:ASN:O	2:B:176:PHE:CE2	2.62	0.52
2:B:312:GLY:CA	2:B:319:TRP:CE2	2.92	0.52
1:A:269:TRP:O	1:A:467:TYR:OH	2.22	0.52
4:D:17:DC:H2''	4:D:18:DT:C5'	2.40	0.52
1:A:98:ASP:O	1:A:102:ARG:N	2.25	0.52
1:A:279:CYS:SG	1:A:281:LEU:CD2	2.98	0.52
2:B:262:GLN:O	2:B:329:LEU:HD21	2.10	0.52
1:A:449:GLU:HG2	1:A:450:ALA:N	2.23	0.52
1:A:33:LEU:HB2	1:A:269:TRP:HA	1.90	0.52
2:B:85:LYS:O	2:B:88:LEU:HD23	2.10	0.52
2:B:249:GLY:HA2	2:B:258:ASN:ND2	2.22	0.52
2:B:337:VAL:HG11	2:B:381:ILE:HD11	1.91	0.52
4:D:11:DT:H2''	4:D:12:DA:O5'	2.10	0.52
1:A:50:LEU:HD11	1:A:91:ILE:HG21	1.92	0.52
1:A:63:PRO:HG3	2:B:124:TRP:CE2	2.45	0.52
1:A:406:MET:HB3	2:B:416:TYR:CD2	2.45	0.51
2:B:330:TYR:CD2	2:B:331:PRO:HA	2.45	0.51
3:C:15:DG:N2	4:D:7:DA:C2	2.78	0.51
3:C:1:DT:C2'	3:C:2:DG:H5'	2.31	0.51
1:A:109:SER:O	1:A:113:ARG:HB3	2.10	0.51
2:B:390:ALA:HB1	2:B:403:ILE:O	2.11	0.51
2:B:17:PHE:CD1	2:B:17:PHE:C	2.84	0.51
2:B:45:PHE:O	2:B:49:ILE:HG13	2.10	0.51
4:D:7:DA:C6	4:D:8:DA:C2	2.98	0.51
2:B:173:SER:OG	2:B:174:ASN:N	2.44	0.51
2:B:265:ILE:O	2:B:269:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:VAL:CG1	2:B:295:ILE:HG12	2.38	0.51
2:B:308:ILE:HG13	2:B:379:ALA:HB2	1.92	0.51
2:B:309:LYS:O	2:B:319:TRP:HH2	1.93	0.51
3:C:17:DA:H2'	3:C:18:DT:C5	2.45	0.51
1:A:371:ASN:HA	1:A:374:ASN:HB2	1.91	0.51
1:A:110:THR:HA	1:A:113:ARG:HE	1.76	0.51
1:A:122:ASN:HD21	1:A:213:ARG:HB3	1.76	0.51
3:C:18:DT:H2''	3:C:19:DA:C8	2.47	0.50
2:B:321:PHE:HD1	2:B:380:PHE:HD2	1.59	0.50
3:C:10:DA:H2'	3:C:11:DG:C1'	2.42	0.50
1:A:80:ALA:HB1	2:B:20:TRP:CZ2	2.46	0.50
2:B:66:THR:N	2:B:103:LEU:HD11	2.27	0.50
2:B:393:LEU:HD11	2:B:403:ILE:HD11	1.93	0.50
1:A:396:LEU:CB	1:A:405:ILE:HD13	2.42	0.50
2:B:5:ILE:N	2:B:31:GLU:O	2.44	0.50
4:D:5:DA:H2''	4:D:6:DC:O5'	2.11	0.50
2:B:21:LEU:O	2:B:25:LEU:HG	2.12	0.50
2:B:97:LEU:CD2	2:B:118:ILE:HG21	2.41	0.50
2:B:267:GLN:OE1	2:B:267:GLN:N	2.41	0.50
2:B:328:LYS:HD2	2:B:336:MET:HE1	1.92	0.50
2:B:332:SER:O	2:B:334:VAL:HG13	2.12	0.50
2:B:158:PHE:CD1	2:B:158:PHE:N	2.78	0.49
2:B:380:PHE:HE1	2:B:384:LEU:HD21	1.77	0.49
1:A:288:ILE:HD13	1:A:491:THR:HG23	1.94	0.49
1:A:329:HIS:CG	1:A:366:ASN:ND2	2.80	0.49
1:A:423:LEU:HG	1:A:434:SER:HB2	1.94	0.49
2:B:295:ILE:HG13	2:B:380:PHE:CE2	2.46	0.49
2:B:323:ILE:HD12	2:B:337:VAL:HG13	1.94	0.49
2:B:408:LEU:HD12	2:B:408:LEU:H	1.77	0.49
1:A:142:ILE:O	1:A:144:PRO:HD3	2.12	0.49
1:A:349:GLN:HB3	1:A:350:ASN:ND2	2.27	0.49
1:A:481:ARG:HH12	4:D:19:DC:P	2.36	0.49
2:B:310:LEU:CD2	2:B:376:LYS:HB3	2.43	0.49
1:A:336:LYS:O	1:A:340:THR:OG1	2.30	0.49
2:B:253:THR:OG1	2:B:256:ILE:O	2.17	0.49
2:B:354:LYS:H	2:B:354:LYS:CD	2.23	0.49
2:B:88:LEU:HG	2:B:90:ASP:HB3	1.94	0.49
2:B:112:ILE:HA	2:B:115:LEU:HD12	1.93	0.49
3:C:15:DG:C2	3:C:16:DT:C2	3.01	0.49
1:A:363:THR:O	1:A:387:THR:OG1	2.27	0.49
2:B:8:SER:HB2	2:B:60:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ASP:N	2:B:35:ASP:OD1	2.45	0.49
3:C:17:DA:C2'	3:C:18:DT:C6	2.95	0.49
2:B:191:ASP:H	2:B:194:LEU:HD23	1.76	0.49
2:B:206:PRO:HB2	2:B:268:LEU:HD23	1.94	0.49
1:A:52:ILE:CG2	1:A:229:LEU:HB2	2.43	0.48
1:A:52:ILE:HG23	1:A:230:ALA:HB2	1.94	0.48
2:B:387:ASP:OD1	2:B:388:GLN:N	2.46	0.48
3:C:17:DA:H2'	3:C:18:DT:C6	2.48	0.48
1:A:390:LYS:NZ	1:A:476:GLU:HG2	2.25	0.48
1:A:468:ASN:OD1	1:A:507:ILE:HG21	2.14	0.48
1:A:501:LEU:HD13	1:A:506:TYR:HE2	1.78	0.48
2:B:9:HIS:CG	2:B:18:THR:HG21	2.48	0.48
2:B:268:LEU:O	2:B:272:ALA:N	2.32	0.48
2:B:308:ILE:HG21	2:B:376:LYS:HA	1.94	0.48
2:B:344:THR:HA	2:B:351:ILE:HG12	1.96	0.48
3:C:4:DG:O6	4:D:16:DC:N4	2.46	0.48
1:A:372:ALA:O	1:A:376:VAL:HG23	2.14	0.48
2:B:350:LEU:HD13	2:B:350:LEU:N	2.27	0.48
4:D:17:DC:H4'	4:D:18:DT:OP1	2.12	0.48
1:A:275:ARG:NH2	1:A:356:GLU:OE2	2.46	0.48
2:B:308:ILE:HG22	2:B:309:LYS:N	2.28	0.48
4:D:18:DT:H2''	4:D:19:DC:C5	2.48	0.48
1:A:321:TYR:HD2	1:A:322:ASN:H	1.61	0.48
2:B:181:PHE:HZ	2:B:269:ILE:HD11	1.79	0.48
2:B:186:ARG:HG3	2:B:188:HIS:CE1	2.49	0.48
2:B:188:HIS:O	2:B:214:LEU:N	2.45	0.48
3:C:4:DG:N2	4:D:18:DT:C2	2.82	0.48
1:A:206:PHE:CZ	1:A:210:LEU:HD12	2.48	0.48
2:B:129:GLN:O	2:B:133:ASP:HB2	2.13	0.48
2:B:178:ILE:HD13	2:B:403:ILE:HG23	1.96	0.48
2:B:36:ILE:HG22	2:B:37:LEU:HD13	1.95	0.48
3:C:11:DG:H2'	3:C:12:DG:C4	2.49	0.48
1:A:236:ASN:HB3	1:A:242:ILE:HG12	1.94	0.48
2:B:69:ASN:OD1	2:B:112:ILE:HD11	2.13	0.48
3:C:9:DT:H2''	3:C:10:DA:O4'	2.13	0.48
1:A:501:LEU:HB2	1:A:506:TYR:CE2	2.48	0.47
2:B:175:TRP:HB2	2:B:408:LEU:CD1	2.44	0.47
3:C:4:DG:H2'	3:C:5:DG:H8	1.76	0.47
4:D:7:DA:N6	4:D:8:DA:N1	2.62	0.47
1:A:71:THR:O	1:A:429:LEU:HD22	2.14	0.47
1:A:132:ASP:HB3	1:A:134:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LYS:HD3	1:A:507:ILE:O	2.14	0.47
1:A:339:LEU:HD22	1:A:339:LEU:HA	1.70	0.47
1:A:463:THR:HB	1:A:474:ASP:N	2.28	0.47
2:B:294:TRP:CB	2:B:342:ILE:HG13	2.43	0.47
1:A:150:TYR:CD2	1:A:157:LEU:HB2	2.48	0.47
1:A:217:HIS:H	1:A:217:HIS:CD2	2.30	0.47
1:A:396:LEU:HB2	1:A:405:ILE:HD13	1.95	0.47
1:A:422:THR:HG22	1:A:460:LEU:HD12	1.97	0.47
2:B:47:SER:O	2:B:51:LYS:N	2.24	0.47
2:B:342:ILE:HG22	2:B:343:PHE:H	1.79	0.47
1:A:135:ARG:HD2	1:A:135:ARG:HA	1.55	0.47
2:B:165:ILE:O	2:B:167:LYS:N	2.47	0.47
4:D:7:DA:C6	4:D:8:DA:N1	2.83	0.47
1:A:225:ARG:HE	1:A:227:SER:CB	2.24	0.47
2:B:3:ASN:OD1	2:B:3:ASN:N	2.48	0.47
2:B:65:SER:HA	2:B:100:ASP:HB2	1.95	0.47
2:B:344:THR:HG22	2:B:349:ASN:O	2.14	0.47
3:C:11:DG:H5'	3:C:12:DG:OP2	2.14	0.47
3:C:11:DG:H3'	3:C:12:DG:C8	2.50	0.47
1:A:212:ALA:O	1:A:215:LEU:HB2	2.14	0.47
2:B:67:ALA:O	2:B:71:ARG:HB2	2.15	0.47
4:D:6:DC:C2'	4:D:7:DA:C8	2.96	0.47
1:A:66:ASN:HD21	1:A:251:HIS:N	2.12	0.47
1:A:357:VAL:O	1:A:383:LEU:HD12	2.15	0.47
1:A:504:LYS:HE3	1:A:505:TYR:CZ	2.50	0.47
2:B:8:SER:OG	2:B:74:VAL:HG13	2.14	0.47
2:B:178:ILE:HA	2:B:403:ILE:HG23	1.95	0.47
2:B:200:VAL:HA	2:B:203:LEU:HD23	1.96	0.47
2:B:285:TYR:HB3	2:B:292:ALA:HB3	1.97	0.47
1:A:30:PHE:HZ	2:B:151:ASN:HB3	1.80	0.47
1:A:40:LYS:HB3	1:A:136:VAL:HA	1.95	0.47
1:A:150:TYR:CE2	1:A:157:LEU:HA	2.49	0.47
2:B:296:GLU:CB	2:B:348:ILE:HG22	2.45	0.47
1:A:27:LEU:O	1:A:31:GLY:N	2.44	0.47
1:A:332:PRO:HD3	1:A:368:GLU:OE1	2.15	0.47
4:D:2:DT:C1'	4:D:3:DA:C8	2.90	0.47
2:B:176:PHE:O	2:B:403:ILE:HG22	2.15	0.47
3:C:14:DT:H3	4:D:7:DA:N6	1.96	0.46
1:A:66:ASN:N	1:A:66:ASN:ND2	2.61	0.46
1:A:398:LYS:HA	2:B:171:TYR:HD1	1.80	0.46
2:B:14:ASP:CG	2:B:63:VAL:HG11	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:DG:C6	3:C:9:DT:C4	3.02	0.46
1:A:329:HIS:CG	1:A:366:ASN:HD22	2.33	0.46
1:A:281:LEU:HD13	1:A:303:MET:HA	1.97	0.46
3:C:18:DT:C2'	3:C:19:DA:C8	2.98	0.46
2:B:178:ILE:H	2:B:178:ILE:HG12	1.34	0.46
2:B:206:PRO:HD2	2:B:395:VAL:O	2.16	0.46
2:B:312:GLY:HA3	2:B:319:TRP:CZ2	2.50	0.46
2:B:393:LEU:HD11	2:B:403:ILE:CD1	2.46	0.46
1:A:15:ALA:HB2	1:A:32:PRO:O	2.15	0.46
1:A:319:PRO:HD2	1:A:320:TRP:CZ3	2.50	0.46
1:A:411:TYR:O	1:A:419:PHE:N	2.37	0.46
1:A:478:VAL:HA	1:A:481:ARG:HB3	1.98	0.46
2:B:7:ILE:HG21	2:B:18:THR:HG22	1.98	0.46
1:A:150:TYR:HE2	1:A:157:LEU:HA	1.80	0.46
2:B:213:TYR:N	2:B:213:TYR:CD2	2.84	0.46
2:B:225:HIS:C	2:B:225:HIS:CD2	2.89	0.46
2:B:258:ASN:O	2:B:262:GLN:HG3	2.16	0.46
4:D:13:DC:H2''	4:D:14:DT:OP2	2.16	0.46
1:A:313:PHE:CZ	1:A:342:ALA:HA	2.50	0.46
1:A:366:ASN:ND2	1:A:369:GLU:OE2	2.49	0.46
1:A:394:LEU:HD21	2:B:410:PHE:CZ	2.50	0.46
2:B:2:ARG:H	2:B:2:ARG:NH1	2.04	0.46
2:B:18:THR:O	2:B:22:SER:OG	2.34	0.46
1:A:21:THR:HG21	1:A:472:TYR:OH	2.16	0.46
1:A:351:LYS:N	1:A:351:LYS:HD2	2.31	0.46
1:A:425:PHE:CE1	1:A:427:PRO:HA	2.51	0.46
1:A:501:LEU:HB2	1:A:506:TYR:HE2	1.80	0.46
1:A:297:ALA:O	1:A:320:TRP:CD1	2.68	0.45
1:A:304:PHE:HZ	1:A:503:PHE:CZ	2.33	0.45
1:A:462:LEU:HD23	1:A:465:LEU:HD12	1.98	0.45
2:B:174:ASN:O	2:B:176:PHE:CD2	2.69	0.45
2:B:343:PHE:HB2	2:B:357:GLN:NE2	2.29	0.45
4:D:10:DC:H1'	4:D:11:DT:H5'	1.98	0.45
1:A:392:LYS:N	1:A:393:PRO:HD3	2.31	0.45
2:B:10:ALA:HA	2:B:71:ARG:HD3	1.97	0.45
1:A:333:LYS:HA	1:A:333:LYS:HD2	1.76	0.45
1:A:393:PRO:HB2	2:B:175:TRP:CZ2	2.50	0.45
1:A:57:LEU:HD21	1:A:86:TRP:CE2	2.52	0.45
1:A:267:LYS:HB2	1:A:467:TYR:CZ	2.52	0.45
2:B:263:ARG:NH1	2:B:263:ARG:HB2	2.32	0.45
1:A:425:PHE:HZ	1:A:430:GLN:CD	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:LEU:HA	2:B:21:LEU:HD12	1.69	0.45
2:B:307:LYS:HB3	2:B:307:LYS:HE2	1.78	0.45
1:A:504:LYS:HA	1:A:507:ILE:CD1	2.46	0.45
2:B:200:VAL:O	2:B:203:LEU:HB2	2.17	0.45
1:A:281:LEU:CB	1:A:359:ILE:HG12	2.47	0.45
1:A:397:TYR:CE1	1:A:437:VAL:HG11	2.52	0.45
1:A:34:ASN:N	1:A:34:ASN:OD1	2.49	0.45
1:A:279:CYS:SG	1:A:303:MET:HG3	2.57	0.45
2:B:22:SER:O	2:B:26:ILE:N	2.42	0.45
2:B:177:PRO:CA	2:B:334:VAL:HG12	2.45	0.45
2:B:308:ILE:HG22	2:B:309:LYS:H	1.81	0.45
2:B:310:LEU:HD23	2:B:376:LYS:HB3	1.99	0.45
2:B:326:ALA:O	2:B:336:MET:N	2.44	0.45
1:A:405:ILE:HG22	2:B:171:TYR:CE1	2.52	0.44
1:A:421:TRP:NE1	1:A:440:PRO:HD3	2.32	0.44
1:A:498:THR:HB	1:A:501:LEU:HD11	1.99	0.44
2:B:255:PHE:CE2	2:B:256:ILE:HG23	2.52	0.44
2:B:371:ASP:N	2:B:371:ASP:OD1	2.49	0.44
3:C:11:DG:H2'	3:C:12:DG:C8	2.52	0.44
1:A:425:PHE:HZ	1:A:430:GLN:OE1	2.00	0.44
2:B:132:LEU:O	2:B:135:PHE:N	2.51	0.44
1:A:332:PRO:HB3	1:A:372:ALA:HB2	1.98	0.44
2:B:345:MET:N	2:B:351:ILE:HD11	2.32	0.44
2:B:1:MET:HA	2:B:2:ARG:NH1	2.32	0.44
1:A:13:LEU:O	1:A:33:LEU:HD12	2.16	0.44
1:A:303:MET:HB2	1:A:313:PHE:HE2	1.82	0.44
1:A:460:LEU:HD12	1:A:460:LEU:HA	1.76	0.44
1:A:476:GLU:O	1:A:477:PRO:C	2.56	0.44
1:A:507:ILE:HG22	1:A:507:ILE:OXT	2.18	0.44
2:B:81:ALA:O	2:B:85:LYS:HB2	2.17	0.44
2:B:270:ASN:HD22	2:B:270:ASN:H	1.65	0.44
2:B:383:PHE:HD1	2:B:384:LEU:HD23	1.83	0.44
1:A:3:GLU:HA	2:B:411:PHE:O	2.18	0.43
1:A:10:PRO:CG	1:A:461:ALA:HA	2.48	0.43
1:A:210:LEU:HD23	1:A:214:LEU:HD12	1.99	0.43
1:A:277:GLY:HA2	1:A:346:TYR:OH	2.17	0.43
2:B:243:THR:HA	2:B:246:ILE:CG1	2.48	0.43
2:B:369:TRP:HA	2:B:369:TRP:CE3	2.53	0.43
4:D:7:DA:C2'	4:D:8:DA:H5''	2.48	0.43
1:A:148:TYR:CD2	4:D:20:DA:C2	3.06	0.43
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:TYR:CE2	2:B:377:LEU:HD22	2.54	0.43
1:A:481:ARG:HH22	4:D:18:DT:H3'	1.83	0.43
2:B:179:ILE:HD12	2:B:390:ALA:HB2	1.99	0.43
2:B:242:SER:O	2:B:245:ASP:HB2	2.18	0.43
1:A:391:SER:O	1:A:393:PRO:HD3	2.19	0.43
3:C:16:DT:H3	4:D:5:DA:H61	1.66	0.43
4:D:18:DT:H2''	4:D:19:DC:C6	2.53	0.43
1:A:80:ALA:N	2:B:125:ALA:HB2	2.32	0.43
1:A:121:PHE:O	1:A:125:ILE:N	2.47	0.43
1:A:328:TYR:O	1:A:329:HIS:ND1	2.52	0.43
2:B:3:ASN:OD1	2:B:56:ASN:ND2	2.51	0.43
2:B:219:TRP:HB3	2:B:221:TYR:CE2	2.53	0.43
1:A:12:ILE:HG13	1:A:14:PHE:CZ	2.54	0.43
1:A:118:VAL:HG13	1:A:210:LEU:HA	2.01	0.43
1:A:339:LEU:O	1:A:343:LEU:HG	2.19	0.43
1:A:388:ILE:HD12	1:A:480:LEU:HD11	1.99	0.43
2:B:50:GLU:O	2:B:54:ARG:HB2	2.18	0.43
1:A:312:VAL:HG11	1:A:506:TYR:CE1	2.54	0.43
2:B:247:LEU:HD12	2:B:248:SER:N	2.34	0.43
2:B:368:TRP:HE3	2:B:373:TRP:CD1	2.37	0.43
1:A:324:GLU:HG3	4:D:8:DA:H3'	2.00	0.43
2:B:263:ARG:O	2:B:267:GLN:OE1	2.37	0.43
1:A:27:LEU:HD21	1:A:268:PRO:HB3	2.01	0.43
1:A:23:PRO:O	1:A:27:LEU:HD12	2.19	0.43
1:A:390:LYS:CE	1:A:476:GLU:CD	2.78	0.43
2:B:270:ASN:HD22	2:B:270:ASN:N	2.16	0.43
2:B:191:ASP:N	2:B:194:LEU:HD23	2.34	0.42
3:C:5:DG:C2	3:C:6:DT:C2	3.07	0.42
2:B:251:TYR:O	2:B:258:ASN:HB2	2.20	0.42
2:B:318:TYR:N	2:B:344:THR:O	2.52	0.42
1:A:398:LYS:CE	1:A:403:PHE:O	2.64	0.42
2:B:266:VAL:HG12	2:B:270:ASN:ND2	2.35	0.42
2:B:341:ILE:HD13	2:B:364:GLN:HG3	2.02	0.42
2:B:245:ASP:HB3	2:B:250:ARG:HB2	2.02	0.42
2:B:248:SER:HB3	2:B:250:ARG:HG2	2.01	0.42
2:B:308:ILE:HD12	2:B:375:GLU:HB2	2.01	0.42
1:A:12:ILE:HG21	1:A:464:LYS:HB3	2.02	0.42
1:A:280:TYR:O	1:A:303:MET:HA	2.18	0.42
2:B:209:ARG:HB3	2:B:209:ARG:NH2	2.33	0.42
1:A:304:PHE:CE1	1:A:479:THR:HA	2.54	0.42
2:B:44:ASP:OD2	2:B:48:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:DG:N2	4:D:11:DT:C2	2.86	0.42
1:A:283:LEU:HA	1:A:283:LEU:HD23	1.44	0.42
1:A:388:ILE:HD13	1:A:477:PRO:HG3	2.01	0.42
1:A:404:PRO:HA	2:B:370:ASN:OD1	2.19	0.42
3:C:9:DT:C2'	3:C:10:DA:C8	3.03	0.42
1:A:98:ASP:HA	1:A:101:ILE:HB	2.01	0.42
1:A:152:ARG:HD3	4:D:20:DA:N1	2.35	0.42
2:B:413:LYS:O	2:B:414:MET:HB2	2.19	0.42
1:A:33:LEU:N	1:A:268:PRO:O	2.52	0.42
1:A:429:LEU:O	1:A:430:GLN:HB2	2.20	0.42
2:B:151:ASN:HA	2:B:154:TYR:HB3	2.01	0.42
1:A:50:LEU:HD21	1:A:93:PHE:CD2	2.52	0.42
1:A:140:PHE:HA	1:A:222:GLN:O	2.20	0.42
1:A:354:PRO:HG2	1:A:357:VAL:CG2	2.50	0.42
1:A:463:THR:CB	1:A:474:ASP:HB3	2.46	0.42
2:B:127:GLY:HA2	2:B:130:ASP:HB2	2.01	0.42
2:B:379:ALA:CA	2:B:382:ARG:HD2	2.48	0.42
3:C:7:DA:H2''	3:C:8:DG:O4'	2.20	0.42
2:B:213:TYR:H	2:B:213:TYR:HD2	1.68	0.41
3:C:10:DA:H2'	3:C:11:DG:H1'	2.02	0.41
1:A:433:LEU:HA	1:A:433:LEU:HD23	1.76	0.41
2:B:41:LYS:HG2	2:B:41:LYS:O	2.19	0.41
1:A:218:THR:O	1:A:219:ILE:HG13	2.20	0.41
2:B:309:LYS:HZ3	2:B:312:GLY:HA3	1.85	0.41
1:A:481:ARG:NH2	4:D:18:DT:H3'	2.35	0.41
2:B:203:LEU:HD12	2:B:223:PHE:CD1	2.50	0.41
2:B:322:GLY:O	2:B:340:HIS:N	2.46	0.41
1:A:9:GLU:HG2	1:A:21:THR:HG21	2.02	0.41
1:A:31:GLY:HA2	1:A:81:VAL:O	2.21	0.41
1:A:295:GLN:HG2	1:A:321:TYR:O	2.21	0.41
1:A:338:LEU:HA	1:A:338:LEU:HD12	1.74	0.41
1:A:428:LYS:HG2	2:B:159:LEU:HD21	2.03	0.41
1:A:465:LEU:HD23	1:A:465:LEU:HA	1.90	0.41
2:B:391:ILE:HG22	2:B:392:TYR:N	2.34	0.41
1:A:50:LEU:HD12	1:A:54:LYS:HG3	2.03	0.41
2:B:311:VAL:HG13	2:B:320:HIS:ND1	2.35	0.41
2:B:323:ILE:HD12	2:B:337:VAL:CG1	2.51	0.41
1:A:22:ASP:HB3	1:A:25:ASP:HB2	2.02	0.41
1:A:404:PRO:HD2	1:A:425:PHE:HB2	2.02	0.41
1:A:248:ILE:O	1:A:251:HIS:HB3	2.21	0.41
1:A:335:ALA:HB1	1:A:373:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ALA:O	1:A:464:LYS:HB2	2.21	0.41
1:A:493:SER:O	1:A:496:ILE:HD11	2.21	0.41
2:B:354:LYS:O	2:B:357:GLN:N	2.53	0.41
2:B:377:LEU:O	2:B:378:LEU:C	2.59	0.41
4:D:7:DA:C3'	4:D:8:DA:H5''	2.51	0.41
1:A:417:LYS:HD3	1:A:444:GLU:HG3	2.02	0.41
2:B:158:PHE:N	2:B:158:PHE:HD1	2.18	0.41
1:A:29:LEU:HB3	1:A:30:PHE:CD1	2.56	0.40
1:A:110:THR:O	1:A:114:THR:N	2.44	0.40
1:A:255:THR:HG23	1:A:469:ALA:HA	2.02	0.40
1:A:274:ILE:HG23	1:A:274:ILE:O	2.21	0.40
2:B:175:TRP:HB2	2:B:408:LEU:HD11	2.03	0.40
2:B:236:GLN:O	2:B:238:SER:N	2.54	0.40
1:A:33:LEU:CD1	1:A:270:LYS:HB2	2.52	0.40
1:A:93:PHE:CE2	1:A:95:GLU:HA	2.54	0.40
1:A:149:LYS:HD2	1:A:149:LYS:HA	1.39	0.40
1:A:390:LYS:CE	1:A:476:GLU:HG3	2.37	0.40
2:B:266:VAL:O	2:B:270:ASN:ND2	2.41	0.40
1:A:42:GLY:N	1:A:136:VAL:HG11	2.37	0.40
1:A:275:ARG:H	1:A:275:ARG:HD3	1.86	0.40
1:A:458:ASP:OD1	1:A:458:ASP:N	2.54	0.40
1:A:36:ILE:HG12	1:A:261:TYR:CE2	2.56	0.40
1:A:134:GLU:O	1:A:135:ARG:HD2	2.21	0.40
1:A:443:ILE:HD13	1:A:459:ILE:HD12	2.03	0.40
2:B:273:PHE:CE1	2:B:325:ALA:HB2	2.57	0.40
2:B:85:LYS:NZ	2:B:91:ASP:O	2.47	0.40
2:B:201:ARG:HH11	2:B:201:ARG:HD2	1.71	0.40
2:B:318:TYR:HE2	2:B:346:ASP:HA	1.85	0.40
2:B:377:LEU:O	2:B:380:PHE:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:LYS:NZ	3:C:18:DT:OP1[2_654]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	470/507 (93%)	437 (93%)	29 (6%)	4 (1%)	14	51
2	B	417/421 (99%)	369 (88%)	42 (10%)	6 (1%)	9	41
All	All	887/928 (96%)	806 (91%)	71 (8%)	10 (1%)	12	47

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	166	GLU
1	A	391	SER
2	B	414	MET
1	A	393	PRO
2	B	195	PRO
2	B	306	GLU
2	B	189	ARG
1	A	310	GLY
2	B	49	ILE
1	A	323	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%)	347 (84%)	67 (16%)	2	10
2	B	372/387 (96%)	291 (78%)	81 (22%)	1	5
All	All	786/833 (94%)	638 (81%)	148 (19%)	1	7

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	56	TYR
1	A	58	ASP
1	A	65	TYR
1	A	68	ASN
1	A	84	CYS
1	A	85	LYS
1	A	88	SER
1	A	97	THR
1	A	113	ARG
1	A	123	ASP
1	A	131	ASN
1	A	132	ASP
1	A	134	GLU
1	A	137	ASP
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	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	299	CYS

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Mol	Chain	Res	Type
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	417	LYS
1	A	423	LEU
1	A	442	PHE
1	A	480	LEU
1	A	493	SER
1	A	494	THR
1	A	497	LYS
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	40	ASP
2	B	45	PHE
2	B	51	LYS
2	B	54	ARG
2	B	56	ASN
2	B	71	ARG
2	B	76	LYS

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Mol	Chain	Res	Type
2	B	78	LEU
2	B	83	LYS
2	B	87	HIS
2	B	88	LEU
2	B	92	MET
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	148	SER
2	B	153	LEU
2	B	154	TYR
2	B	159	LEU
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
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	227	LEU
2	B	239	ILE
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	300	LEU
2	B	302	LYS

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Mol	Chain	Res	Type
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	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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	122	ASN
1	A	163	GLN
1	A	217	HIS
1	A	350	ASN
1	A	366	ASN
1	A	430	GLN
1	A	468	ASN
2	B	56	ASN
2	B	138	GLN
2	B	188	HIS
2	B	197	GLN
2	B	225	HIS
2	B	270	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	474/507 (93%)	-0.83	0 100 100	493, 540, 620, 678	0
2	B	419/421 (99%)	-0.78	1 (0%) 92 85	494, 571, 636, 665	0
3	C	21/21 (100%)	-0.40	0 100 100	546, 599, 647, 666	0
4	D	20/20 (100%)	-0.31	0 100 100	532, 609, 650, 653	0
All	All	934/969 (96%)	-0.79	1 (0%) 92 88	493, 557, 635, 678	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	112	ILE	2.7

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(Å ²)	Q<0.9
5	MG	D	101	1/1	0.94	0.04	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.