



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:56 AM UTC

PDB ID : 2Y9Z / pdb_00002y9z
Title : Chromatin Remodeling Factor ISW1a(del_ATPase) in DNA complex
Authors : Yamada, K.; Frouws, T.D.; Angst, B.; Fitzgerald, D.J.; DeLuca, C.; Schim-
mele, K.; Sargent, D.F.; Richmond, T.J.
Deposited on : 2011-02-17
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

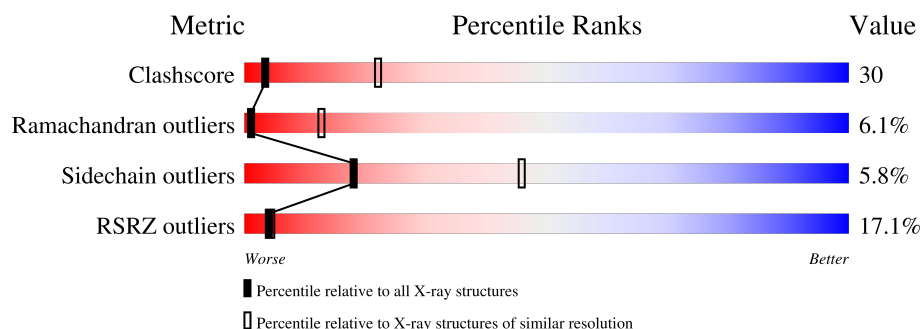
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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))
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	374	10% 34% 39% 23%
2	B	624	13% 38% 48% 8% 5%
3	C	48	42% 40% 25% 35%
3	D	48	35% 25% 40% 35%
3	E	48	15% 25% 23% 52%
3	F	48	6% 21% 27% 52%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9500 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 IMITATION SWITCH PROTEIN 1 (DEL_ATPASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2404	1524	417	454	9			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	762	MET	-	expression tag	UNP P38144
A	1130	HIS	-	expression tag	UNP P38144
A	1131	HIS	-	expression tag	UNP P38144
A	1132	HIS	-	expression tag	UNP P38144
A	1133	HIS	-	expression tag	UNP P38144
A	1134	HIS	-	expression tag	UNP P38144
A	1135	HIS	-	expression tag	UNP P38144

- Molecule 2 is a protein called ISWI ONE COMPLEX PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	595	Total	C	N	O	S	0	0	0
			4882	3140	823	904	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	126	MET	-	expression tag	UNP P43596

- Molecule 3 is a DNA chain called I-DNA/E-DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	P	0	0	0
			635	303	117	184	31			
3	D	31	Total	C	N	O	P	0	0	0
			636	304	113	188	31			

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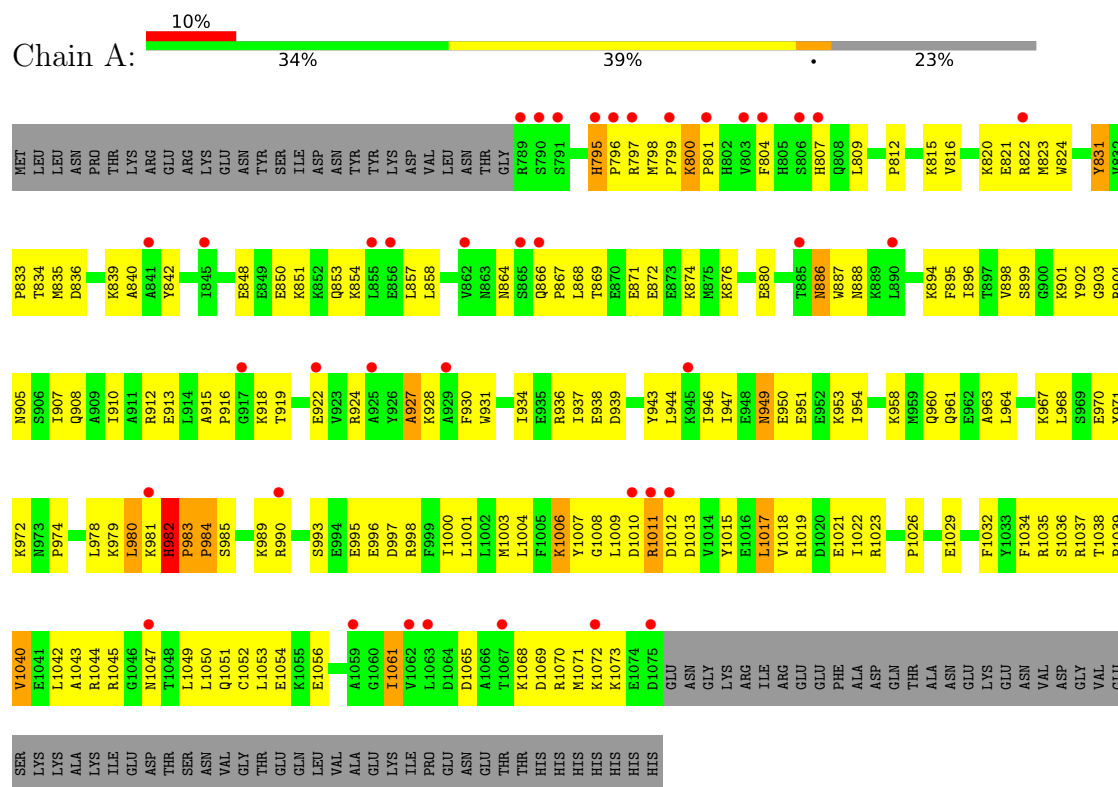
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	23	Total	C	N	O	P	0	0	0
			475	226	86	140	23			
3	F	23	Total	C	N	O	P	0	0	0
			468	223	86	136	23			

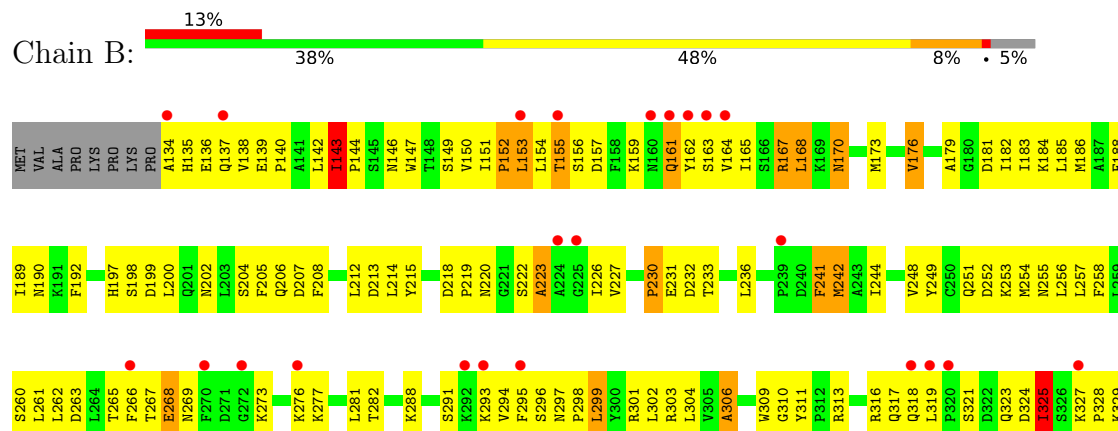
3 Residue-property plots

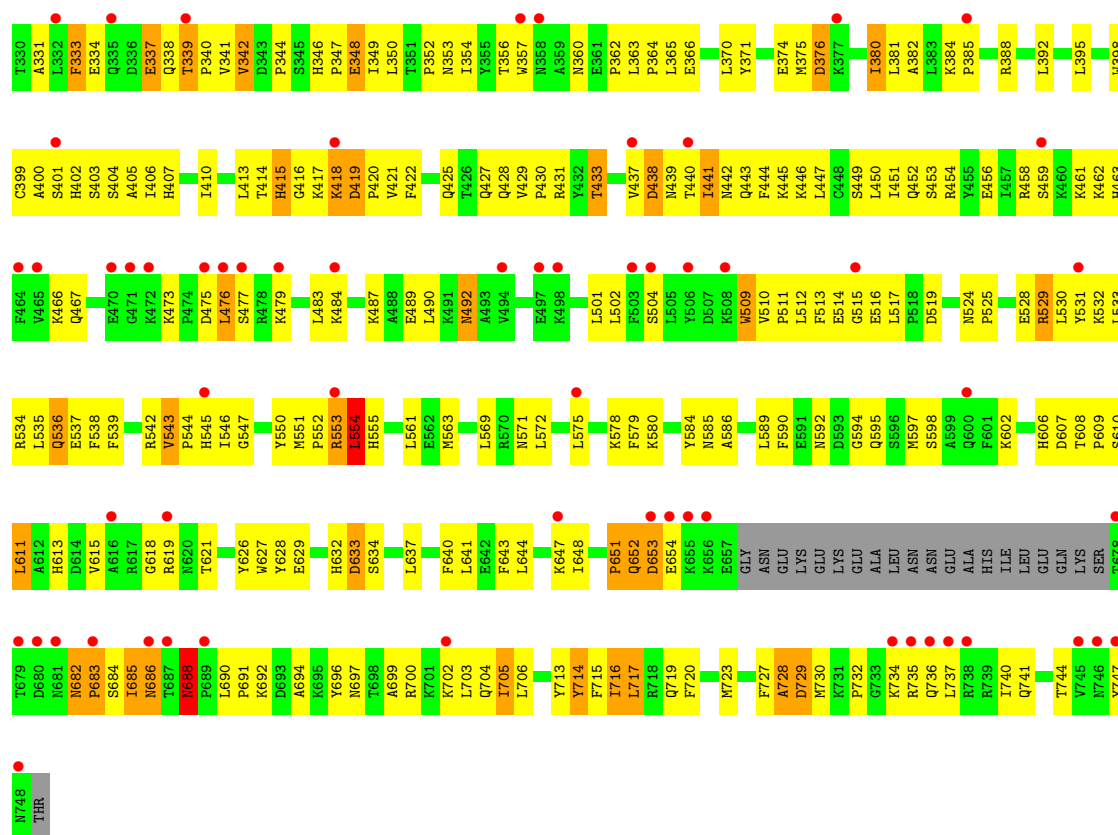
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: IMITATION SWITCH PROTEIN 1 (DEL_ATPASE)



• Molecule 2: ISWI ONE COMPLEX PROTEIN 3

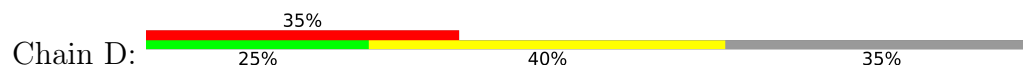




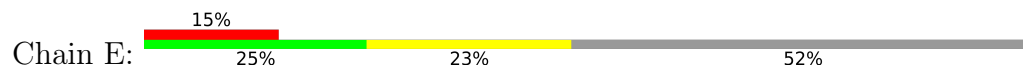
• Molecule 3: I-DNA/E-DNA



• Molecule 3: I-DNA/E-DNA



• Molecule 3: I-DNA/E-DNA



• Molecule 3: I-DNA/E-DNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	284.03Å 284.03Å 193.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.95 – 3.60 29.95 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.95-3.60) 99.6 (29.95-3.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 3.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.283 , 0.291 0.281 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	118.1	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 137.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9500	wwPDB-VP
Average B, all atoms (Å ²)	172.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/2455	0.71	0/3297
2	B	0.30	0/5005	0.72	6/6769 (0.1%)
3	C	0.13	0/712	0.49	0/1096
3	D	0.13	0/712	0.49	0/1097
3	E	0.16	0/532	0.59	0/820
3	F	0.16	0/524	0.54	0/805
All	All	0.26	0/9940	0.67	6/13884 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	547	GLY	N-CA-C	5.64	118.39	110.38
2	B	143	ILE	CA-C-N	5.13	124.30	118.97
2	B	143	ILE	C-N-CA	5.13	124.30	118.97
2	B	419	ASP	CA-C-N	5.09	125.38	119.93
2	B	419	ASP	C-N-CA	5.09	125.38	119.93
2	B	167	ARG	N-CA-C	-5.06	107.16	113.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2404	0	2394	169	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4882	0	4870	340	0
3	C	635	0	350	13	0
3	D	636	0	352	19	0
3	E	475	0	261	16	3
3	F	468	0	259	11	3
All	All	9500	0	8486	542	3

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 30.

All (542) 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)
2:B:327:LYS:HG3	2:B:328:PRO:HD3	1.27	1.17
1:A:795:HIS:HB2	1:A:796:PRO:HD3	1.46	0.98
1:A:886:ASN:HD22	1:A:887:TRP:H	1.12	0.95
1:A:869:THR:HG22	1:A:871:GLU:H	1.32	0.95
1:A:1015:TYR:CD2	1:A:1043:ALA:HA	2.04	0.92
3:D:28:DC:H2"	3:D:29:DT:H5"	1.54	0.88
2:B:475:ASP:HB3	2:B:479:LYS:HD3	1.57	0.86
2:B:461:LYS:HZ2	2:B:463:HIS:H	1.25	0.83
1:A:901:LYS:HG2	1:A:950:GLU:HG2	1.60	0.82
2:B:364:PRO:HB2	2:B:366:GLU:HG2	1.64	0.80
1:A:919:THR:HG22	1:A:922:GLU:HG2	1.63	0.79
2:B:176:VAL:HG13	2:B:179:ALA:HB2	1.64	0.79
1:A:1003:MET:HE1	2:B:619:ARG:HD2	1.64	0.79
3:E:40:DT:H3	3:F:9:DA:H61	1.28	0.79
2:B:150:VAL:O	2:B:430:PRO:HA	1.84	0.78
2:B:586:ALA:HB2	2:B:719:GLN:HG3	1.66	0.77
1:A:886:ASN:ND2	1:A:887:TRP:H	1.82	0.77
2:B:554:LEU:HG	2:B:598:SER:H	1.48	0.77
2:B:268:GLU:HB2	2:B:404:SER:HB2	1.67	0.77
3:D:14:DT:H2"	3:D:15:DA:H5"	1.67	0.77
2:B:339:THR:HB	2:B:340:PRO:HD3	1.67	0.76
2:B:445:LYS:HB3	2:B:445:LYS:HZ3	1.51	0.75
2:B:611:LEU:HD23	2:B:626:TYR:CZ	2.23	0.73
1:A:982:HIS:C	1:A:984:PRO:HD3	2.12	0.73
2:B:293:LYS:HB3	2:B:296:SER:HB3	1.70	0.73
1:A:886:ASN:HD22	1:A:887:TRP:N	1.86	0.73
2:B:147:TRP:HH2	2:B:446:LYS:HD2	1.55	0.72
1:A:1019:ARG:HH12	2:B:310:GLY:HA3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:ASP:O	2:B:184:LYS:HB3	1.89	0.72
2:B:144:PRO:HB2	2:B:421:VAL:HG21	1.70	0.71
2:B:329:LYS:HB3	2:B:356:THR:O	1.90	0.71
2:B:551:MET:HE1	2:B:717:LEU:HD21	1.70	0.71
3:E:27:DG:H2'	3:E:28:DC:H6	1.55	0.71
1:A:908:GLN:OE1	2:B:334:GLU:HG2	1.91	0.70
3:C:19:DA:H5'	3:C:19:DA:H8	1.55	0.70
3:E:27:DG:H2'	3:E:28:DC:C6	2.25	0.70
1:A:904:ARG:HH22	1:A:931:TRP:HE1	1.39	0.70
2:B:543:VAL:HG13	2:B:546:ILE:HB	1.74	0.70
1:A:799:PRO:HB3	1:A:822:ARG:HH21	1.56	0.70
2:B:554:LEU:HG	2:B:598:SER:N	2.07	0.70
1:A:869:THR:HB	1:A:872:GLU:HG3	1.74	0.69
1:A:833:PRO:HG2	1:A:858:LEU:HA	1.74	0.69
2:B:682:ASN:C	2:B:684:SER:H	2.00	0.69
2:B:563:MET:HE2	2:B:592:ASN:HB2	1.73	0.69
2:B:134:ALA:HB1	2:B:138:VAL:HG23	1.75	0.68
2:B:260:SER:HA	2:B:282:THR:HG21	1.76	0.68
2:B:149:SER:OG	2:B:519:ASP:HB3	1.93	0.68
1:A:981:LYS:HA	1:A:984:PRO:HG3	1.74	0.67
2:B:147:TRP:CD2	2:B:447:LEU:HD12	2.29	0.67
1:A:950:GLU:O	1:A:954:ILE:HD13	1.94	0.67
2:B:219:PRO:C	2:B:220:ASN:HD22	2.03	0.67
2:B:197:HIS:H	2:B:200:LEU:HD12	1.60	0.67
2:B:325:ILE:HB	2:B:328:PRO:HD2	1.77	0.67
1:A:928:LYS:HA	2:B:342:VAL:HG23	1.77	0.66
2:B:205:PHE:CD1	2:B:602:LYS:HG3	2.30	0.66
1:A:797:ARG:C	1:A:799:PRO:HD3	2.20	0.66
2:B:218:ASP:HB3	2:B:222:SER:O	1.94	0.66
2:B:319:LEU:HD13	2:B:324:ASP:HB2	1.77	0.66
2:B:297:ASN:HB3	2:B:298:PRO:HD3	1.78	0.66
1:A:807:HIS:CE1	1:A:937:ILE:HG23	2.31	0.66
2:B:327:LYS:CG	2:B:328:PRO:HD3	2.17	0.66
2:B:461:LYS:HD3	2:B:462:LYS:N	2.10	0.66
2:B:154:LEU:N	2:B:154:LEU:HD12	2.11	0.65
2:B:437:VAL:O	2:B:440:THR:HG22	1.95	0.65
3:D:12:DC:H2''	3:D:13:DG:C8	2.31	0.65
1:A:1003:MET:HB3	1:A:1018:VAL:HG12	1.77	0.65
2:B:489:GLU:HA	2:B:492:ASN:HB2	1.79	0.65
2:B:580:LYS:HA	2:B:715:PHE:CD2	2.32	0.65
2:B:578:LYS:HD3	2:B:584:TYR:CE2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:LEU:HD11	1:A:937:ILE:HG12	1.77	0.65
1:A:824:TRP:CE3	1:A:867:PRO:HG3	2.32	0.65
2:B:147:TRP:CG	2:B:447:LEU:HD12	2.32	0.65
2:B:544:PRO:HD3	2:B:702:LYS:HD2	1.79	0.65
1:A:1045:ARG:O	1:A:1049:LEU:HD23	1.96	0.64
2:B:578:LYS:HD3	2:B:584:TYR:HE2	1.63	0.64
2:B:594:GLY:C	2:B:723:MET:HE1	2.23	0.64
1:A:876:LYS:O	1:A:880:GLU:HG2	1.97	0.64
1:A:982:HIS:CB	1:A:983:PRO:HD3	2.28	0.64
1:A:834:THR:HA	1:A:854:LYS:HE2	1.80	0.63
1:A:807:HIS:HE1	1:A:937:ILE:HG23	1.63	0.63
1:A:919:THR:HG22	1:A:922:GLU:CG	2.28	0.63
1:A:903:GLY:HA2	2:B:350:LEU:HB2	1.81	0.63
3:C:19:DA:H5'	3:C:19:DA:C8	2.33	0.63
2:B:150:VAL:HA	2:B:431:ARG:HB2	1.81	0.62
2:B:554:LEU:HD12	2:B:598:SER:OG	2.00	0.62
1:A:1071:MET:HG3	1:A:1072:LYS:N	2.15	0.62
1:A:1061:ILE:HD13	1:A:1061:ILE:O	2.00	0.62
2:B:509:TRP:CD1	2:B:512:LEU:HD12	2.35	0.62
1:A:1000:ILE:O	1:A:1004:LEU:HG	2.00	0.62
2:B:136:GLU:OE1	2:B:461:LYS:HE2	1.99	0.62
1:A:997:ASP:O	1:A:1000:ILE:HG12	2.00	0.62
2:B:705:ILE:HG13	2:B:706:LEU:N	2.14	0.62
1:A:823:MET:HE1	1:A:857:LEU:HD21	1.82	0.62
2:B:162:TYR:HB3	2:B:613:HIS:CD2	2.35	0.62
2:B:323:GLN:HG3	2:B:324:ASP:OD1	1.99	0.62
1:A:799:PRO:HB3	1:A:822:ARG:NH2	2.15	0.61
2:B:188:PHE:O	2:B:192:PHE:HD1	1.83	0.61
2:B:410:ILE:O	2:B:414:THR:HG22	2.00	0.61
1:A:981:LYS:NZ	1:A:990:ARG:HH12	1.98	0.61
2:B:263:ASP:HB2	2:B:282:THR:CG2	2.31	0.61
1:A:907:ILE:O	1:A:910:ILE:HG12	2.00	0.61
2:B:199:ASP:HB3	2:B:253:LYS:HE2	1.83	0.61
3:C:12:DC:H2''	3:C:13:DG:N7	2.15	0.61
1:A:961:GLN:HA	1:A:1009:LEU:HD23	1.83	0.61
2:B:350:LEU:O	2:B:352:PRO:HD3	2.01	0.60
1:A:982:HIS:HB2	1:A:983:PRO:HD3	1.83	0.60
2:B:164:VAL:HG13	2:B:607:ASP:OD2	2.00	0.60
1:A:915:ALA:HB3	1:A:916:PRO:HD3	1.82	0.60
2:B:595:GLN:N	2:B:723:MET:HE1	2.17	0.60
1:A:980:LEU:HA	1:A:982:HIS:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:ILE:HG22	2:B:186:MET:HE2	1.83	0.60
2:B:611:LEU:HD23	2:B:626:TYR:CE1	2.37	0.60
1:A:983:PRO:N	1:A:984:PRO:HD3	2.15	0.60
2:B:329:LYS:HD2	2:B:329:LYS:N	2.17	0.60
1:A:993:SER:HG	1:A:996:GLU:H	1.48	0.60
1:A:797:ARG:HG3	1:A:798:MET:H	1.65	0.59
1:A:905:ASN:HB3	2:B:341:VAL:HB	1.84	0.59
3:E:39:DG:H1	3:F:10:DC:H42	1.49	0.59
2:B:276:LYS:HD2	2:B:281:LEU:HA	1.84	0.59
2:B:331:ALA:HB3	2:B:356:THR:OG1	2.01	0.59
1:A:899:SER:HA	1:A:910:ILE:HG21	1.83	0.59
2:B:170:ASN:HA	2:B:686:ASN:HB3	1.83	0.59
2:B:403:SER:C	2:B:405:ALA:H	2.10	0.59
1:A:824:TRP:CE2	1:A:867:PRO:HB3	2.38	0.59
2:B:329:LYS:HD2	2:B:329:LYS:H	1.67	0.59
1:A:1070:ARG:HH11	1:A:1073:LYS:HD3	1.68	0.58
2:B:154:LEU:HD23	2:B:542:ARG:NH2	2.18	0.58
2:B:157:ASP:C	2:B:159:LYS:N	2.59	0.58
2:B:447:LEU:HD23	2:B:447:LEU:C	2.28	0.58
1:A:982:HIS:ND1	1:A:983:PRO:HD3	2.18	0.58
2:B:417:LYS:O	2:B:418:LYS:HB2	2.02	0.58
1:A:868:LEU:HA	1:A:872:GLU:OE1	2.04	0.58
2:B:744:THR:HA	2:B:747:TYR:HB3	1.85	0.57
1:A:947:ILE:O	1:A:951:GLU:HG3	2.04	0.57
3:D:17:DA:H2''	3:D:18:DT:H5'	1.86	0.57
1:A:918:LYS:HG2	1:A:922:GLU:HG3	1.86	0.57
2:B:606:HIS:CD2	2:B:627:TRP:CE2	2.93	0.57
1:A:930:PHE:CZ	1:A:934:ILE:HD13	2.40	0.57
2:B:152:PRO:O	2:B:153:LEU:HB3	2.04	0.57
2:B:218:ASP:HB3	2:B:223:ALA:HB2	1.87	0.57
2:B:266:PHE:CZ	2:B:302:LEU:HA	2.39	0.57
2:B:265:THR:HG22	2:B:399:CYS:HA	1.85	0.57
3:E:25:DA:H2''	3:E:26:DG:H8	1.69	0.57
2:B:339:THR:CB	2:B:340:PRO:HD3	2.34	0.56
2:B:425:GLN:O	2:B:534:ARG:HG2	2.05	0.56
3:E:40:DT:H3	3:F:9:DA:N6	2.00	0.56
1:A:954:ILE:HG21	2:B:350:LEU:HD23	1.87	0.56
2:B:461:LYS:HD3	2:B:461:LYS:C	2.30	0.56
2:B:154:LEU:C	2:B:156:SER:H	2.12	0.56
2:B:741:GLN:O	2:B:744:THR:HG22	2.06	0.56
3:E:25:DA:H2''	3:E:26:DG:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:LYS:HE2	1:A:913:GLU:HG2	1.88	0.56
1:A:896:ILE:HG13	1:A:947:ILE:HD11	1.88	0.56
2:B:690:LEU:HG	2:B:691:PRO:HD2	1.88	0.56
3:C:35:DA:H2'	3:C:36:DC:C6	2.40	0.56
2:B:476:LEU:HD21	2:B:515:GLY:HA3	1.88	0.55
3:C:11:DC:H2''	3:C:12:DC:H5'	1.88	0.55
1:A:848:GLU:O	1:A:851:LYS:HG2	2.06	0.55
2:B:563:MET:HE3	2:B:589:LEU:HA	1.87	0.55
1:A:1003:MET:SD	1:A:1021:GLU:HG2	2.47	0.55
2:B:648:ILE:HG21	2:B:704:GLN:HG2	1.88	0.55
2:B:140:PRO:HB2	2:B:450:LEU:HD11	1.89	0.54
2:B:606:HIS:ND1	2:B:608:THR:HG23	2.21	0.54
2:B:403:SER:C	2:B:405:ALA:N	2.64	0.54
1:A:904:ARG:NH2	1:A:931:TRP:HE1	2.06	0.54
1:A:1019:ARG:NH1	1:A:1023:ARG:HH21	2.05	0.54
2:B:135:HIS:HD2	2:B:136:GLU:HG3	1.72	0.54
3:E:26:DG:H2''	3:E:27:DG:O4'	2.06	0.54
1:A:981:LYS:HZ3	1:A:990:ARG:HH12	1.53	0.54
2:B:165:ILE:O	2:B:165:ILE:HD12	2.07	0.54
3:D:11:DC:H2'	3:D:12:DC:C6	2.42	0.54
1:A:1015:TYR:HA	1:A:1018:VAL:HG22	1.88	0.54
1:A:1019:ARG:HH11	1:A:1023:ARG:HH21	1.55	0.54
2:B:151:ILE:HG13	2:B:531:TYR:CG	2.42	0.54
1:A:960:GLN:HB3	1:A:1050:LEU:HD12	1.90	0.54
1:A:1001:LEU:HD11	1:A:1049:LEU:HD12	1.88	0.54
2:B:244:ILE:O	2:B:248:VAL:HG23	2.08	0.54
2:B:447:LEU:O	2:B:451:ILE:HG22	2.08	0.54
1:A:797:ARG:HD3	1:A:831:TYR:HD2	1.73	0.54
2:B:694:ALA:HA	2:B:697:ASN:ND2	2.23	0.54
2:B:413:LEU:HD22	2:B:533:LEU:HB2	1.90	0.53
1:A:904:ARG:HD2	1:A:951:GLU:OE1	2.09	0.53
1:A:1044:ARG:NH1	3:D:28:DC:H4'	2.23	0.53
2:B:159:LYS:HA	2:B:161:GLN:HE22	1.73	0.53
1:A:816:VAL:O	1:A:820:LYS:HG2	2.09	0.53
2:B:143:ILE:HG13	2:B:146:ASN:H	1.74	0.53
2:B:212:LEU:HD11	2:B:254:MET:HE2	1.89	0.53
3:C:37:DG:H2''	3:C:38:DG:H5'	1.89	0.53
2:B:473:LYS:HB2	2:B:476:LEU:HB2	1.91	0.53
1:A:1036:SER:C	1:A:1037:ARG:HD2	2.32	0.53
2:B:375:MET:O	2:B:376:ASP:C	2.51	0.53
2:B:329:LYS:HG2	2:B:357:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:682:ASN:N	2:B:683:PRO:CD	2.72	0.53
2:B:337:GLU:OE1	2:B:353:ASN:HB2	2.09	0.53
2:B:475:ASP:C	2:B:477:SER:H	2.16	0.53
2:B:715:PHE:HD1	2:B:715:PHE:H	1.55	0.53
1:A:1037:ARG:NH1	2:B:410:ILE:HD11	2.24	0.53
2:B:208:PHE:O	2:B:212:LEU:HD12	2.08	0.53
2:B:163:SER:C	2:B:165:ILE:H	2.18	0.52
2:B:218:ASP:CB	2:B:223:ALA:HB2	2.39	0.52
2:B:682:ASN:H	2:B:683:PRO:CD	2.21	0.52
1:A:967:LYS:CD	1:A:971:TYR:HE2	2.22	0.52
1:A:1068:LYS:HE3	1:A:1070:ARG:HH21	1.75	0.52
2:B:152:PRO:HD2	2:B:429:VAL:O	2.10	0.52
2:B:441:ILE:HG13	2:B:442:ASN:N	2.24	0.52
2:B:713:TYR:O	2:B:714:TYR:C	2.53	0.52
3:F:18:DT:H1'	3:F:19:DA:H5''	1.91	0.52
2:B:157:ASP:C	2:B:159:LYS:H	2.16	0.52
2:B:420:PRO:HG3	2:B:530:LEU:HD12	1.92	0.52
2:B:483:LEU:HD22	2:B:487:LYS:HE3	1.92	0.52
3:C:10:DC:N4	3:D:39:DG:H1	2.08	0.52
3:F:7:DG:H2''	3:F:8:DA:C8	2.45	0.52
2:B:682:ASN:C	2:B:684:SER:N	2.66	0.52
3:E:32:DT:H2''	3:E:33:DA:C5'	2.40	0.52
1:A:795:HIS:CB	1:A:796:PRO:HD3	2.28	0.52
2:B:414:THR:HG23	2:B:415:HIS:N	2.25	0.51
1:A:866:GLN:N	1:A:867:PRO:HD3	2.25	0.51
1:A:958:LYS:O	1:A:961:GLN:HB3	2.09	0.51
2:B:291:SER:O	2:B:294:VAL:HG23	2.10	0.51
3:C:26:DG:H1	3:D:23:DC:H42	1.58	0.51
2:B:249:TYR:CZ	2:B:253:LYS:HE3	2.45	0.51
2:B:321:SER:HB2	2:B:323:GLN:HG2	1.91	0.51
2:B:696:TYR:O	2:B:700:ARG:HG3	2.09	0.51
1:A:850:GLU:HA	1:A:853:GLN:HB2	1.90	0.51
1:A:983:PRO:HG2	1:A:1052:CYS:O	2.10	0.51
2:B:406:ILE:O	2:B:410:ILE:HG23	2.10	0.51
2:B:151:ILE:HA	2:B:429:VAL:O	2.11	0.51
2:B:553:ARG:C	2:B:554:LEU:HD13	2.35	0.51
2:B:538:PHE:CD1	2:B:552:PRO:HA	2.46	0.51
2:B:142:LEU:HD21	2:B:516:GLU:HB3	1.93	0.51
2:B:159:LYS:HA	2:B:161:GLN:NE2	2.26	0.51
2:B:688:ASN:N	2:B:688:ASN:ND2	2.59	0.51
3:E:28:DC:H3'	3:E:29:DT:H71	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:GLN:HB2	2:B:363:LEU:HD13	1.92	0.50
2:B:154:LEU:C	2:B:156:SER:N	2.70	0.50
2:B:441:ILE:O	2:B:444:PHE:HB3	2.11	0.50
1:A:807:HIS:C	1:A:809:LEU:H	2.20	0.50
2:B:154:LEU:HD11	2:B:429:VAL:HG13	1.93	0.50
2:B:479:LYS:HE3	2:B:512:LEU:HA	1.93	0.50
2:B:572:LEU:HD13	2:B:572:LEU:C	2.36	0.50
2:B:590:PHE:HE1	2:B:595:GLN:HE21	1.58	0.50
2:B:144:PRO:HA	2:B:517:LEU:HD22	1.94	0.50
2:B:162:TYR:HD1	2:B:613:HIS:CE1	2.30	0.50
2:B:261:LEU:O	2:B:265:THR:HG23	2.12	0.50
2:B:590:PHE:HE1	2:B:595:GLN:NE2	2.10	0.50
1:A:871:GLU:O	1:A:874:LYS:HB3	2.12	0.49
2:B:288:LYS:O	2:B:288:LYS:HG3	2.12	0.49
2:B:299:LEU:HD22	2:B:303:ARG:CZ	2.42	0.49
2:B:398:TRP:O	2:B:402:HIS:HD2	1.96	0.49
1:A:1036:SER:O	1:A:1037:ARG:HD2	2.13	0.49
2:B:143:ILE:HD12	2:B:144:PRO:HD2	1.94	0.49
2:B:428:GLN:HG3	2:B:534:ARG:HB3	1.94	0.49
1:A:972:LYS:H	1:A:972:LYS:HD2	1.78	0.49
1:A:1026:PRO:O	1:A:1029:GLU:HG3	2.12	0.49
2:B:346:HIS:C	2:B:348:GLU:H	2.20	0.49
1:A:797:ARG:HD3	1:A:831:TYR:CD2	2.47	0.49
3:C:36:DC:O5'	3:C:36:DC:H6	1.96	0.49
1:A:799:PRO:HA	1:A:822:ARG:NE	2.28	0.49
2:B:414:THR:HG23	2:B:415:HIS:H	1.77	0.49
1:A:1068:LYS:HE3	1:A:1070:ARG:NH2	2.28	0.49
2:B:555:HIS:HD2	2:B:597:MET:HE1	1.77	0.49
1:A:980:LEU:H	1:A:980:LEU:HD22	1.77	0.49
2:B:487:LYS:O	2:B:490:LEU:HB2	2.13	0.49
2:B:589:LEU:HD21	2:B:720:PHE:CD1	2.47	0.49
3:C:18:DT:H2''	3:C:19:DA:H5'	1.94	0.49
2:B:318:GLN:O	2:B:319:LEU:C	2.55	0.49
3:D:36:DC:H2''	3:D:37:DG:OP1	2.13	0.49
2:B:452:GLN:HE21	2:B:487:LYS:HE2	1.77	0.49
2:B:452:GLN:HG3	2:B:487:LYS:HE2	1.94	0.48
2:B:555:HIS:CD2	2:B:597:MET:HE1	2.48	0.48
1:A:799:PRO:O	1:A:800:LYS:HB3	2.13	0.48
2:B:168:LEU:HD13	2:B:173:MET:SD	2.53	0.48
1:A:807:HIS:O	1:A:809:LEU:HD22	2.13	0.48
2:B:648:ILE:HD13	2:B:704:GLN:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:VAL:O	2:B:150:VAL:HG22	2.14	0.48
2:B:168:LEU:HD12	2:B:168:LEU:H	1.78	0.48
2:B:273:LYS:O	2:B:273:LYS:HG2	2.13	0.48
2:B:380:ILE:O	2:B:380:ILE:HD13	2.13	0.48
2:B:651:PRO:C	2:B:653:ASP:H	2.20	0.48
1:A:809:LEU:HD22	1:A:809:LEU:N	2.29	0.48
2:B:161:GLN:HE21	2:B:161:GLN:N	2.12	0.48
2:B:374:GLU:HB2	2:B:382:ALA:HB1	1.95	0.48
2:B:302:LEU:HD22	2:B:370:LEU:HD21	1.95	0.48
2:B:325:ILE:HB	2:B:328:PRO:CD	2.41	0.48
2:B:438:ASP:O	2:B:441:ILE:HG13	2.14	0.48
2:B:139:GLU:OE2	2:B:458:ARG:HD3	2.14	0.48
2:B:370:LEU:HD13	2:B:370:LEU:O	2.14	0.48
1:A:901:LYS:C	1:A:903:GLY:H	2.21	0.47
1:A:815:LYS:HD3	1:A:815:LYS:C	2.39	0.47
1:A:1049:LEU:O	1:A:1052:CYS:HB2	2.14	0.47
2:B:139:GLU:HB3	2:B:454:ARG:HG3	1.95	0.47
2:B:407:HIS:O	2:B:410:ILE:HG13	2.14	0.47
2:B:542:ARG:O	2:B:702:LYS:HD3	2.14	0.47
2:B:652:GLN:C	2:B:654:GLU:H	2.22	0.47
2:B:299:LEU:HD13	2:B:303:ARG:HH12	1.79	0.47
1:A:1038:THR:O	1:A:1042:LEU:HB3	2.15	0.47
1:A:1070:ARG:HD2	1:A:1070:ARG:N	2.29	0.47
2:B:555:HIS:HD2	2:B:597:MET:SD	2.38	0.47
2:B:647:LYS:HD2	2:B:647:LYS:N	2.30	0.47
1:A:967:LYS:HD2	1:A:971:TYR:HE2	1.78	0.47
1:A:1015:TYR:HD2	1:A:1042:LEU:HD23	1.79	0.47
2:B:146:ASN:HD22	2:B:146:ASN:C	2.21	0.47
2:B:536:GLN:NE2	2:B:550:TYR:HE2	2.12	0.47
2:B:569:LEU:C	2:B:569:LEU:HD13	2.40	0.47
2:B:251:GLN:O	2:B:252:ASP:C	2.55	0.47
2:B:346:HIS:O	2:B:348:GLU:N	2.48	0.47
2:B:528:GLU:O	2:B:529:ARG:C	2.58	0.47
2:B:433:THR:HG21	2:B:539:PHE:HD2	1.80	0.46
2:B:543:VAL:HG21	2:B:546:ILE:HD12	1.97	0.46
3:E:32:DT:H2''	3:E:33:DA:O5'	2.15	0.46
2:B:269:ASN:N	2:B:269:ASN:HD22	2.13	0.46
2:B:430:PRO:HD3	2:B:535:LEU:HD11	1.98	0.46
3:D:12:DC:H2''	3:D:13:DG:H8	1.78	0.46
1:A:963:ALA:HB1	1:A:1053:LEU:HD22	1.98	0.46
2:B:241:PHE:HB3	2:B:242:MET:H	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:972:LYS:O	1:A:974:PRO:HD3	2.15	0.46
2:B:306:ALA:HB1	2:B:311:TYR:CE1	2.50	0.46
1:A:857:LEU:HD13	1:A:857:LEU:O	2.15	0.46
2:B:293:LYS:HB3	2:B:296:SER:CB	2.44	0.46
2:B:555:HIS:HD2	2:B:597:MET:CE	2.29	0.46
2:B:350:LEU:HD12	2:B:350:LEU:H	1.81	0.46
1:A:928:LYS:CA	2:B:342:VAL:HG23	2.46	0.46
1:A:1003:MET:HA	1:A:1006:LYS:HB2	1.97	0.46
2:B:453:SER:HA	2:B:456:GLU:HG2	1.97	0.46
3:C:10:DC:H42	3:D:39:DG:H1	1.63	0.46
3:D:16:DT:H2''	3:D:17:DA:H8	1.81	0.46
2:B:317:GLN:O	2:B:318:GLN:C	2.58	0.46
2:B:685:ILE:HD12	2:B:685:ILE:N	2.31	0.46
1:A:1044:ARG:HH12	3:D:28:DC:H4'	1.80	0.45
2:B:212:LEU:HD23	2:B:388:ARG:HB3	1.97	0.45
2:B:571:ASN:O	2:B:575:LEU:HG	2.16	0.45
1:A:1036:SER:HA	2:B:400:ALA:O	2.16	0.45
2:B:302:LEU:C	2:B:302:LEU:HD23	2.42	0.45
1:A:1015:TYR:CE2	1:A:1043:ALA:HA	2.49	0.45
1:A:1039:PRO:O	1:A:1043:ALA:HB2	2.17	0.45
2:B:149:SER:CB	2:B:519:ASP:HB3	2.47	0.45
2:B:640:PHE:O	2:B:643:PHE:HB3	2.16	0.45
1:A:982:HIS:CG	1:A:983:PRO:HD3	2.52	0.45
2:B:189:ILE:HD11	2:B:257:LEU:HD11	1.97	0.45
2:B:266:PHE:O	2:B:268:GLU:HG3	2.17	0.45
3:D:13:DG:H8	3:D:13:DG:OP2	2.00	0.45
2:B:553:ARG:HD2	2:B:554:LEU:HD13	1.97	0.45
2:B:641:LEU:O	2:B:644:LEU:HB2	2.17	0.45
3:F:23:DC:H2''	3:F:24:DT:O5'	2.17	0.45
2:B:212:LEU:HD11	2:B:254:MET:HG3	1.99	0.45
2:B:606:HIS:HB2	2:B:627:TRP:CZ3	2.52	0.45
2:B:651:PRO:HG2	2:B:692:LYS:HB3	1.99	0.45
1:A:995:GLU:O	1:A:996:GLU:C	2.60	0.45
2:B:365:LEU:HD22	2:B:371:TYR:CE2	2.52	0.45
2:B:627:TRP:C	2:B:628:TYR:CD1	2.95	0.45
2:B:585:ASN:OD1	2:B:586:ALA:N	2.48	0.45
2:B:608:THR:N	2:B:609:PRO:CD	2.80	0.45
1:A:821:GLU:O	1:A:822:ARG:C	2.60	0.45
1:A:968:LEU:C	1:A:970:GLU:H	2.23	0.45
1:A:1007:TYR:HB3	2:B:357:TRP:CH2	2.52	0.45
2:B:173:MET:HA	2:B:629:GLU:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:THR:HG22	2:B:399:CYS:SG	2.57	0.45
3:F:14:DT:H2"	3:F:15:DA:H8	1.80	0.45
2:B:182:ILE:O	2:B:185:LEU:HB2	2.17	0.45
2:B:608:THR:OG1	2:B:609:PRO:HD3	2.16	0.45
3:E:37:DG:H2"	3:E:38:DG:H8	1.81	0.45
2:B:301:ARG:HA	2:B:304:LEU:HD12	1.97	0.44
2:B:384:LYS:O	2:B:385:PRO:C	2.60	0.44
2:B:530:LEU:N	2:B:530:LEU:HD23	2.32	0.44
2:B:692:LYS:O	2:B:692:LYS:HG3	2.17	0.44
1:A:918:LYS:HB3	1:A:922:GLU:CB	2.48	0.44
1:A:989:LYS:HD3	1:A:989:LYS:HA	1.67	0.44
1:A:1007:TYR:CD1	1:A:1017:LEU:HD13	2.52	0.44
2:B:153:LEU:C	2:B:154:LEU:HD12	2.42	0.44
3:D:19:DA:H2"	3:D:20:DA:C8	2.52	0.44
2:B:151:ILE:HG13	2:B:531:TYR:CD2	2.53	0.44
2:B:226:ILE:HG12	2:B:236:LEU:O	2.18	0.44
2:B:325:ILE:HD12	2:B:328:PRO:HG2	1.98	0.44
2:B:632:HIS:O	2:B:633:ASP:HB3	2.18	0.44
1:A:797:ARG:HA	1:A:797:ARG:HD2	1.52	0.44
1:A:939:ASP:O	1:A:943:TYR:HD2	2.00	0.44
2:B:206:GLN:O	2:B:207:ASP:C	2.60	0.44
2:B:212:LEU:HD12	2:B:212:LEU:N	2.33	0.44
2:B:734:LYS:HG3	2:B:735:ARG:N	2.32	0.44
1:A:1069:ASP:C	1:A:1070:ARG:HD2	2.42	0.44
2:B:333:PHE:HB3	2:B:334:GLU:H	1.68	0.44
2:B:487:LYS:HA	2:B:490:LEU:HD13	2.00	0.44
2:B:422:PHE:HZ	2:B:428:GLN:HG2	1.83	0.44
2:B:538:PHE:CE1	2:B:553:ARG:N	2.83	0.44
1:A:1006:LYS:O	2:B:327:LYS:HB3	2.18	0.44
1:A:972:LYS:C	1:A:974:PRO:HD3	2.42	0.44
2:B:212:LEU:O	2:B:213:ASP:C	2.60	0.44
2:B:648:ILE:CG2	2:B:704:GLN:HG2	2.48	0.44
1:A:824:TRP:HB2	1:A:864:ASN:ND2	2.33	0.44
2:B:295:PHE:O	2:B:298:PRO:HD2	2.18	0.44
2:B:532:LYS:O	2:B:533:LEU:C	2.60	0.44
2:B:611:LEU:HB2	2:B:626:TYR:CD2	2.52	0.44
2:B:615:VAL:HA	2:B:619:ARG:HA	2.00	0.44
2:B:705:ILE:C	2:B:705:ILE:HD12	2.43	0.44
1:A:974:PRO:O	1:A:978:LEU:HB3	2.18	0.43
2:B:473:LYS:HG3	2:B:476:LEU:HD12	2.00	0.43
2:B:579:PHE:CD1	2:B:716:ILE:HG12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:PHE:CG	1:A:896:ILE:N	2.84	0.43
1:A:1000:ILE:HD11	1:A:1049:LEU:HG	2.00	0.43
1:A:1010:ASP:O	1:A:1011:ARG:C	2.60	0.43
2:B:483:LEU:HB3	2:B:487:LYS:HE3	2.00	0.43
3:D:27:DG:H5'	3:D:27:DG:H8	1.83	0.43
1:A:812:PRO:HG2	1:A:936:ARG:NH1	2.34	0.43
2:B:154:LEU:O	2:B:156:SER:N	2.51	0.43
2:B:163:SER:C	2:B:165:ILE:N	2.76	0.43
2:B:414:THR:C	2:B:416:GLY:H	2.26	0.43
1:A:1054:GLU:C	1:A:1056:GLU:H	2.26	0.43
2:B:167:ARG:NH1	2:B:691:PRO:HG2	2.34	0.43
1:A:834:THR:HG22	1:A:836:ASP:H	1.84	0.43
2:B:197:HIS:N	2:B:200:LEU:HD12	2.30	0.43
2:B:230:PRO:HB2	2:B:231:GLU:H	1.69	0.43
2:B:585:ASN:HA	2:B:719:GLN:HE21	1.84	0.43
2:B:484:LYS:N	2:B:484:LYS:HD2	2.33	0.43
2:B:490:LEU:C	2:B:492:ASN:H	2.25	0.43
3:F:18:DT:H2''	3:F:19:DA:H5'	2.01	0.43
1:A:804:PHE:O	1:A:807:HIS:HB3	2.19	0.43
2:B:183:ILE:HG12	2:B:552:PRO:HG3	2.01	0.43
1:A:798:MET:N	1:A:799:PRO:HD3	2.33	0.43
1:A:1032:PHE:HE2	2:B:188:PHE:HD2	1.67	0.43
2:B:150:VAL:C	2:B:151:ILE:HG12	2.44	0.43
2:B:222:SER:O	2:B:223:ALA:HB2	2.19	0.43
2:B:381:LEU:HA	2:B:388:ARG:NE	2.34	0.43
2:B:483:LEU:HD23	2:B:483:LEU:HA	1.83	0.43
2:B:510:VAL:HB	2:B:511:PRO:HD3	2.00	0.43
2:B:543:VAL:CG2	2:B:546:ILE:HD12	2.49	0.43
2:B:727:PHE:O	2:B:728:ALA:HB2	2.19	0.43
1:A:824:TRP:CZ3	1:A:867:PRO:HG3	2.53	0.43
1:A:979:LYS:HA	1:A:979:LYS:HD2	1.80	0.43
2:B:200:LEU:HD11	2:B:256:LEU:HD12	2.00	0.43
2:B:333:PHE:HB2	2:B:354:ILE:O	2.19	0.43
1:A:1068:LYS:HG3	1:A:1070:ARG:HH21	1.84	0.43
2:B:153:LEU:HD12	2:B:425:GLN:HG2	1.99	0.43
2:B:164:VAL:HG13	2:B:610:SER:HB2	2.01	0.43
2:B:197:HIS:CG	2:B:198:SER:N	2.87	0.43
2:B:212:LEU:HD11	2:B:254:MET:SD	2.59	0.43
2:B:439:ASN:O	2:B:443:GLN:HG2	2.19	0.43
2:B:249:TYR:OH	2:B:253:LYS:HE3	2.18	0.42
2:B:263:ASP:HB2	2:B:282:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:ASP:O	2:B:267:THR:HB	2.19	0.42
2:B:381:LEU:HA	2:B:388:ARG:HE	1.83	0.42
1:A:869:THR:H	1:A:872:GLU:CD	2.27	0.42
1:A:949:ASN:O	1:A:953:LYS:HG3	2.19	0.42
2:B:258:PHE:O	2:B:262:LEU:HG	2.19	0.42
2:B:537:GLU:CD	2:B:537:GLU:H	2.27	0.42
2:B:538:PHE:HE1	2:B:553:ARG:H	1.59	0.42
2:B:651:PRO:C	2:B:653:ASP:N	2.77	0.42
2:B:433:THR:HG21	2:B:539:PHE:CD2	2.55	0.42
2:B:705:ILE:CG1	2:B:706:LEU:N	2.78	0.42
2:B:728:ALA:O	2:B:729:ASP:HB2	2.18	0.42
3:D:34:DT:H6	3:D:34:DT:H2'	1.69	0.42
1:A:824:TRP:CE3	1:A:864:ASN:ND2	2.87	0.42
1:A:1061:ILE:O	1:A:1065:ASP:HB2	2.20	0.42
2:B:197:HIS:ND1	2:B:198:SER:N	2.67	0.42
2:B:276:LYS:CD	2:B:281:LEU:HA	2.49	0.42
2:B:447:LEU:C	2:B:449:SER:N	2.77	0.42
2:B:684:SER:OG	2:B:685:ILE:HD12	2.19	0.42
3:C:10:DC:N3	3:D:39:DG:N2	2.61	0.42
1:A:904:ARG:HH22	1:A:931:TRP:NE1	2.14	0.42
1:A:908:GLN:HG3	2:B:338:GLN:OE1	2.18	0.42
1:A:996:GLU:O	1:A:997:ASP:C	2.63	0.42
2:B:447:LEU:CD2	2:B:513:PHE:HE1	2.32	0.42
2:B:637:LEU:O	2:B:641:LEU:HG	2.19	0.42
1:A:823:MET:HE1	1:A:857:LEU:CD2	2.49	0.42
1:A:1047:ASN:O	1:A:1051:GLN:HG3	2.20	0.42
2:B:342:VAL:O	2:B:344:PRO:HD3	2.19	0.42
1:A:799:PRO:HA	1:A:822:ARG:HG3	2.01	0.42
1:A:984:PRO:HB2	1:A:985:SER:H	1.69	0.42
2:B:155:THR:O	2:B:156:SER:C	2.62	0.42
2:B:456:GLU:HA	2:B:459:SER:HB3	2.02	0.42
2:B:501:LEU:HD12	2:B:502:LEU:N	2.34	0.42
2:B:682:ASN:O	2:B:684:SER:N	2.52	0.42
1:A:938:GLU:O	1:A:939:ASP:HB2	2.19	0.42
1:A:968:LEU:C	1:A:970:GLU:N	2.76	0.42
2:B:154:LEU:N	2:B:154:LEU:CD1	2.80	0.42
2:B:204:SER:HB3	2:B:598:SER:HB2	2.01	0.42
2:B:392:LEU:O	2:B:395:LEU:HB3	2.20	0.42
2:B:466:LYS:HG3	2:B:467:GLN:HG3	2.01	0.42
1:A:898:VAL:HG23	1:A:910:ILE:HB	2.01	0.42
2:B:437:VAL:O	2:B:441:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:ILE:C	2:B:441:ILE:HD12	2.45	0.42
3:E:26:DG:C2	3:E:27:DG:C4	3.07	0.42
3:F:4:DC:H2''	3:F:5:DA:C8	2.55	0.42
3:F:13:DG:H2'	3:F:14:DT:H72	2.02	0.42
1:A:866:GLN:H	1:A:867:PRO:HD3	1.85	0.42
1:A:924:ARG:O	1:A:927:ALA:HB3	2.20	0.42
2:B:184:LYS:O	2:B:185:LEU:C	2.62	0.42
2:B:536:GLN:NE2	2:B:550:TYR:CE2	2.87	0.42
1:A:980:LEU:CA	1:A:982:HIS:CE1	3.02	0.41
2:B:151:ILE:HG21	2:B:531:TYR:CD1	2.55	0.41
2:B:215:TYR:HB2	2:B:223:ALA:O	2.20	0.41
2:B:430:PRO:HB2	2:B:433:THR:OG1	2.20	0.41
1:A:835:MET:HE3	1:A:850:GLU:HB2	2.02	0.41
2:B:429:VAL:HA	2:B:535:LEU:CD1	2.50	0.41
2:B:543:VAL:HG21	2:B:703:LEU:HG	2.01	0.41
2:B:589:LEU:O	2:B:594:GLY:HA3	2.20	0.41
1:A:1006:LYS:HZ2	2:B:619:ARG:HD3	1.85	0.41
1:A:1049:LEU:O	1:A:1050:LEU:C	2.64	0.41
2:B:419:ASP:HA	2:B:420:PRO:HD3	1.95	0.41
1:A:918:LYS:HB3	1:A:922:GLU:HB3	2.02	0.41
1:A:1018:VAL:CG2	1:A:1042:LEU:HD21	2.49	0.41
1:A:1038:THR:C	1:A:1040:VAL:N	2.77	0.41
2:B:153:LEU:N	2:B:153:LEU:HD23	2.35	0.41
3:D:20:DA:H2''	3:D:21:DG:C8	2.55	0.41
3:E:39:DG:H1	3:F:10:DC:N4	2.15	0.41
1:A:1004:LEU:HD13	1:A:1050:LEU:HD21	2.03	0.41
2:B:142:LEU:HD22	2:B:454:ARG:HD3	2.02	0.41
2:B:212:LEU:O	2:B:214:LEU:HG	2.20	0.41
2:B:554:LEU:HG	2:B:597:MET:HA	2.03	0.41
2:B:561:LEU:HD23	2:B:561:LEU:HA	1.89	0.41
2:B:705:ILE:HG13	2:B:706:LEU:H	1.81	0.41
1:A:944:LEU:C	1:A:946:ILE:H	2.29	0.41
1:A:995:GLU:O	1:A:998:ARG:HB2	2.20	0.41
2:B:313:ARG:HA	2:B:316:ARG:CZ	2.51	0.41
2:B:554:LEU:HD23	2:B:555:HIS:N	2.36	0.41
1:A:907:ILE:H	2:B:338:GLN:HE22	1.69	0.41
1:A:996:GLU:O	1:A:1000:ILE:HG23	2.20	0.41
2:B:190:ASN:C	2:B:192:PHE:H	2.28	0.41
2:B:265:THR:HA	2:B:403:SER:OG	2.20	0.41
2:B:364:PRO:C	2:B:366:GLU:N	2.79	0.41
2:B:428:GLN:O	2:B:535:LEU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:553:ARG:HD2	2:B:554:LEU:CD1	2.51	0.41
3:C:17:DA:C5	3:C:18:DT:C4	3.09	0.41
3:E:26:DG:H2'	3:E:27:DG:H8	1.86	0.41
2:B:202:ASN:O	2:B:598:SER:HB3	2.20	0.41
1:A:1022:ILE:HG22	1:A:1035:ARG:HG2	2.03	0.40
1:A:1071:MET:HG3	1:A:1072:LYS:HG2	2.02	0.40
2:B:475:ASP:C	2:B:477:SER:N	2.79	0.40
2:B:736:GLN:O	2:B:737:LEU:C	2.64	0.40
2:B:220:ASN:HD22	2:B:220:ASN:N	2.18	0.40
2:B:697:ASN:C	2:B:699:ALA:N	2.79	0.40
2:B:715:PHE:CD1	2:B:715:PHE:N	2.85	0.40
1:A:1012:ASP:HB3	1:A:1013:ASP:H	1.60	0.40
2:B:463:HIS:CD2	2:B:467:GLN:NE2	2.90	0.40
2:B:510:VAL:N	2:B:511:PRO:CD	2.84	0.40
2:B:652:GLN:HE21	2:B:652:GLN:HB3	1.61	0.40
1:A:869:THR:HB	1:A:872:GLU:CG	2.46	0.40
1:A:1053:LEU:HD23	1:A:1053:LEU:O	2.21	0.40
2:B:579:PHE:CG	2:B:716:ILE:HG12	2.57	0.40
3:E:32:DT:H2''	3:E:33:DA:H5''	2.03	0.40
1:A:839:LYS:HG3	1:A:840:ALA:N	2.35	0.40
2:B:524:ASN:HA	2:B:525:PRO:HD3	1.90	0.40
2:B:545:HIS:CD2	2:B:545:HIS:N	2.90	0.40

All (3) 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)
3:E:25:DA:P	3:F:24:DT:O3'[11_655]	1.68	0.52
3:E:25:DA:OP2	3:F:24:DT:O3'[11_655]	1.83	0.37
3:E:25:DA:O5'	3:F:24:DT:O3'[11_655]	2.11	0.09

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	285/374 (76%)	205 (72%)	69 (24%)	11 (4%)	2	20
2	B	591/624 (95%)	411 (70%)	138 (23%)	42 (7%)	1	10
All	All	876/998 (88%)	616 (70%)	207 (24%)	53 (6%)	1	13

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	801	PRO
1	A	831	TYR
1	A	983	PRO
1	A	984	PRO
2	B	223	ALA
2	B	333	PHE
2	B	492	ASN
2	B	621	THR
1	A	927	ALA
2	B	152	PRO
2	B	155	THR
2	B	230	PRO
2	B	348	GLU
2	B	418	LYS
2	B	529	ARG
2	B	634	SER
2	B	714	TYR
2	B	728	ALA
1	A	795	HIS
1	A	842	TYR
1	A	982	HIS
1	A	1011	ARG
2	B	153	LEU
2	B	242	MET
2	B	339	THR
2	B	362	PRO
2	B	376	ASP
2	B	476	LEU
2	B	618	GLY
2	B	686	ASN
2	B	732	PRO
2	B	740	ILE
2	B	306	ALA
2	B	325	ILE

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Mol	Chain	Res	Type
2	B	504	SER
2	B	688	ASN
1	A	902	TYR
2	B	137	GLN
2	B	241	PHE
2	B	277	LYS
2	B	360	ASN
2	B	415	HIS
2	B	438	ASP
2	B	554	LEU
2	B	633	ASP
2	B	651	PRO
2	B	653	ASP
2	B	683	PRO
2	B	729	ASP
2	B	730	MET
2	B	232	ASP
1	A	1008	GLY
2	B	347	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	264/343 (77%)	251 (95%)	13 (5%)	22	49
2	B	546/571 (96%)	512 (94%)	34 (6%)	16	44
All	All	810/914 (89%)	763 (94%)	47 (6%)	18	46

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	800	LYS
1	A	886	ASN
1	A	888	ASN
1	A	912	ARG

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Mol	Chain	Res	Type
1	A	949	ASN
1	A	964	LEU
1	A	980	LEU
1	A	982	HIS
1	A	1006	LYS
1	A	1017	LEU
1	A	1034	PHE
1	A	1040	VAL
1	A	1061	ILE
2	B	143	ILE
2	B	161	GLN
2	B	168	LEU
2	B	170	ASN
2	B	176	VAL
2	B	227	VAL
2	B	233	THR
2	B	255	ASN
2	B	268	GLU
2	B	299	LEU
2	B	309	TRP
2	B	325	ILE
2	B	337	GLU
2	B	342	VAL
2	B	349	ILE
2	B	380	ILE
2	B	401	SER
2	B	427	GLN
2	B	433	THR
2	B	441	ILE
2	B	509	TRP
2	B	514	GLU
2	B	536	GLN
2	B	543	VAL
2	B	553	ARG
2	B	554	LEU
2	B	611	LEU
2	B	652	GLN
2	B	682	ASN
2	B	685	ILE
2	B	688	ASN
2	B	705	ILE
2	B	716	ILE

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Mol	Chain	Res	Type
2	B	717	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	810	GLN
1	A	863	ASN
1	A	864	ASN
1	A	886	ASN
1	A	905	ASN
1	A	949	ASN
1	A	973	ASN
1	A	982	HIS
1	A	988	ASN
1	A	1058	ASN
2	B	135	HIS
2	B	146	ASN
2	B	161	GLN
2	B	202	ASN
2	B	220	ASN
2	B	251	GLN
2	B	269	ASN
2	B	317	GLN
2	B	318	GLN
2	B	402	HIS
2	B	427	GLN
2	B	442	ASN
2	B	467	GLN
2	B	492	ASN
2	B	536	GLN
2	B	545	HIS
2	B	555	HIS
2	B	582	ASN
2	B	606	HIS
2	B	613	HIS
2	B	632	HIS
2	B	652	GLN
2	B	681	ASN
2	B	682	ASN
2	B	719	GLN
2	B	722	GLN
2	B	741	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	287/374 (76%)	1.10	39 (13%) 7 6	86, 134, 225, 267	0
2	B	595/624 (95%)	1.08	83 (13%) 6 6	73, 120, 216, 286	0
3	C	31/48 (64%)	2.28	20 (64%) 0 0	225, 298, 411, 480	0
3	D	31/48 (64%)	2.12	17 (54%) 0 0	221, 315, 408, 420	0
3	E	23/48 (47%)	1.56	7 (30%) 1 1	118, 237, 356, 404	0
3	F	23/48 (47%)	1.14	3 (13%) 7 6	107, 239, 376, 389	0
All	All	990/1190 (83%)	1.17	169 (17%) 4 4	73, 130, 301, 480	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	746	ASN	7.4
2	B	476	LEU	6.4
2	B	320	PRO	6.2
1	A	803	VAL	5.7
1	A	796	PRO	5.4
1	A	865	SER	5.3
1	A	981	LYS	5.3
2	B	459	SER	5.1
2	B	678	THR	5.1
1	A	855	LEU	4.4
2	B	531	TYR	4.4
1	A	922	GLU	4.4
1	A	866	GLN	4.3
2	B	654	GLU	4.2
2	B	224	ALA	4.2
2	B	270	PHE	4.1
2	B	164	VAL	4.1
2	B	472	LYS	4.0
1	A	797	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	484	LYS	3.9
3	D	39	DG	3.9
3	D	40	DT	3.9
2	B	508	LYS	3.8
2	B	679	THR	3.8
2	B	683	PRO	3.8
2	B	475	ASP	3.8
2	B	553	ARG	3.7
1	A	1059	ALA	3.7
2	B	503	PHE	3.7
2	B	506	TYR	3.6
2	B	332	LEU	3.6
3	C	31	DA	3.5
1	A	925	ALA	3.5
2	B	680	ASP	3.5
2	B	155	THR	3.5
1	A	791	SER	3.4
2	B	327	LYS	3.4
2	B	747	TYR	3.4
1	A	856	GLU	3.4
1	A	1010	ASP	3.4
3	C	14	DT	3.4
1	A	845	ILE	3.3
2	B	653	ASP	3.3
2	B	689	PRO	3.3
2	B	687	THR	3.2
2	B	464	PHE	3.2
1	A	806	SER	3.2
3	D	34	DT	3.2
2	B	292	LYS	3.2
3	C	30	DT	3.2
3	C	35	DA	3.1
1	A	862	VAL	3.1
1	A	807	HIS	3.1
1	A	1072	LYS	3.1
2	B	748	ASN	3.1
3	C	15	DA	3.1
2	B	702	LYS	3.1
3	C	32	DT	3.1
2	B	357	TRP	3.0
3	F	10	DC	3.0
2	B	575	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	619	ARG	3.0
2	B	494	VAL	3.0
2	B	498	LYS	2.9
3	C	10	DC	2.9
3	C	18	DT	2.9
3	C	34	DT	2.9
2	B	497	GLU	2.9
2	B	479	LYS	2.9
1	A	804	PHE	2.9
3	D	31	DA	2.9
1	A	790	SER	2.9
2	B	339	THR	2.9
3	E	44	DT	2.9
1	A	795	HIS	2.8
3	D	41	DT	2.8
2	B	272	GLY	2.8
1	A	1075	ASP	2.8
3	C	12	DC	2.8
2	B	225	GLY	2.8
2	B	686	ASN	2.8
2	B	736	GLN	2.7
1	A	1011	ARG	2.7
2	B	655	LYS	2.7
3	C	33	DA	2.7
3	D	35	DA	2.7
1	A	822	ARG	2.7
1	A	945	LYS	2.7
2	B	734	LYS	2.7
3	C	36	DC	2.7
3	C	38	DG	2.7
1	A	801	PRO	2.7
3	C	25	DA	2.7
3	C	29	DT	2.6
2	B	161	GLN	2.6
2	B	600	GLN	2.6
2	B	745	VAL	2.6
1	A	929	ALA	2.6
3	C	37	DG	2.6
2	B	160	ASN	2.6
2	B	735	ARG	2.6
2	B	276	LYS	2.5
3	E	43	DA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	440	THR	2.5
3	E	41	DT	2.5
1	A	1047	ASN	2.5
3	D	11	DC	2.5
1	A	885	THR	2.5
2	B	134	ALA	2.4
3	D	30	DT	2.4
3	F	2	DC	2.4
2	B	471	GLY	2.4
1	A	890	LEU	2.4
1	A	799	PRO	2.4
3	D	29	DT	2.4
2	B	319	LEU	2.3
3	D	14	DT	2.3
3	C	13	DG	2.3
2	B	293	LYS	2.3
3	E	42	DC	2.3
2	B	163	SER	2.3
3	C	11	DC	2.2
1	A	789	ARG	2.2
2	B	401	SER	2.2
2	B	358	ASN	2.2
2	B	681	ASN	2.2
3	C	16	DT	2.2
3	D	18	DT	2.2
3	D	32	DT	2.2
3	E	46	DC	2.2
2	B	137	GLN	2.2
2	B	318	GLN	2.2
2	B	738	ARG	2.2
2	B	162	TYR	2.2
1	A	1067	THR	2.2
2	B	418	LYS	2.2
2	B	153	LEU	2.2
2	B	504	SER	2.1
3	D	24	DT	2.1
2	B	385	PRO	2.1
2	B	515	GLY	2.1
1	A	1063	LEU	2.1
3	D	38	DG	2.1
3	E	34	DT	2.1
2	B	470	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	737	LEU	2.1
3	F	9	DA	2.1
1	A	1012	ASP	2.1
2	B	545	HIS	2.1
2	B	647	LYS	2.1
2	B	239	PRO	2.1
2	B	477	SER	2.1
3	D	33	DA	2.1
3	D	27	DG	2.1
1	A	990	ARG	2.1
1	A	841	ALA	2.1
2	B	656	LYS	2.1
3	C	20	DA	2.1
3	D	13	DG	2.1
2	B	266	PHE	2.1
2	B	335	GLN	2.1
2	B	465	VAL	2.1
1	A	917	GLY	2.0
2	B	377	LYS	2.0
3	E	33	DA	2.0
1	A	1062	VAL	2.0
2	B	295	PHE	2.0
2	B	616	ALA	2.0
2	B	437	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.