Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 06:52 am BST

PDB ID	:	2Y9Z
Title	:	Chromatin Remodeling Factor ISW1a(del_ATPase) in DNA complex
Authors	:	Yamada, K.; Frouws, T.D.; Angst, B.; Fitzgerald, D.J.; DeLuca, C.; Schimmele, 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:

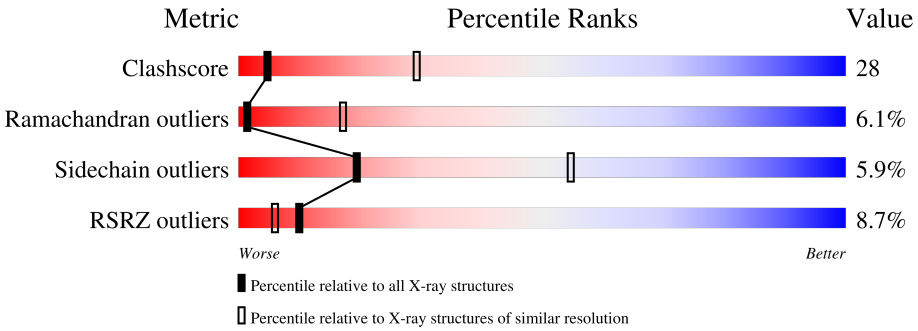
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (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 <=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	5% 36% 37% · 23%
2	B	624	4% 41% 47% 7% · 5%
3	C	48	31% 40% 25% 35%
3	D	48	40% 25% 40% 35%
3	E	48	12% 25% 23% 52%
3	F	48	12% 21% 27% 52%

2 Entry composition (i)

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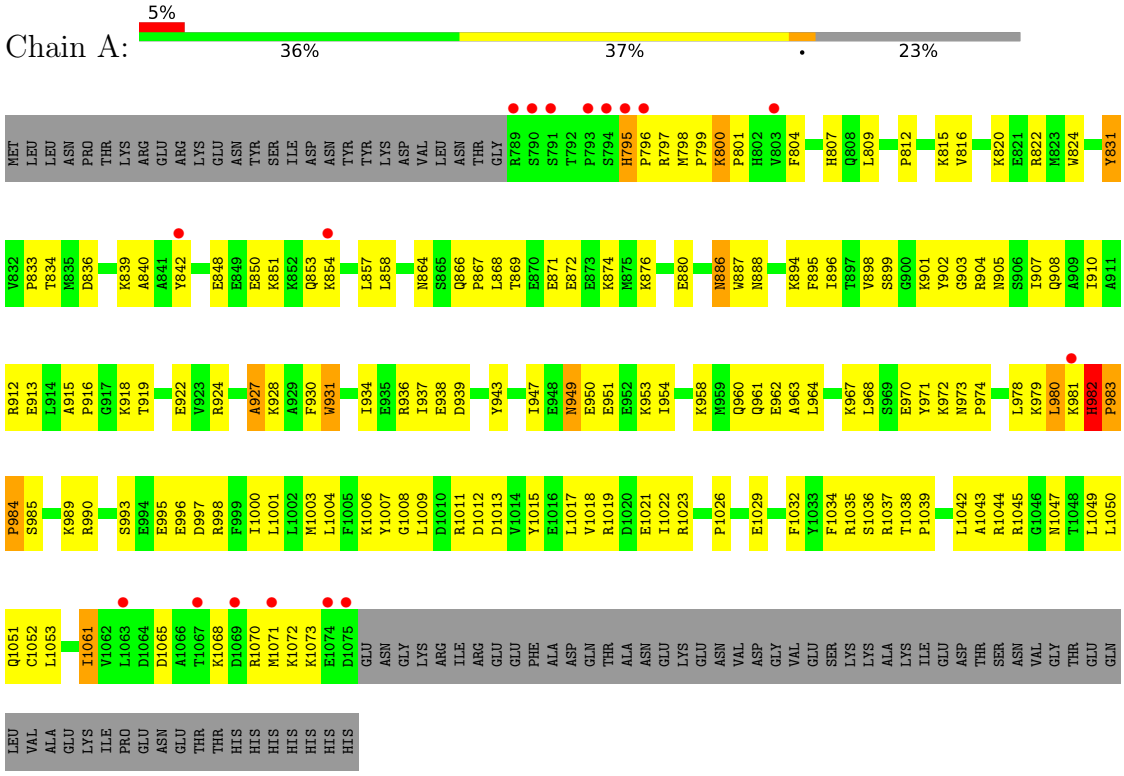
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	23	Total	C	N	O	P	0	0	0
			475	226	86	140	23			
3	F	23	Total	C	N	O	P	0	0	0
			468	223	86	136	23			

3 Residue-property plots (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.

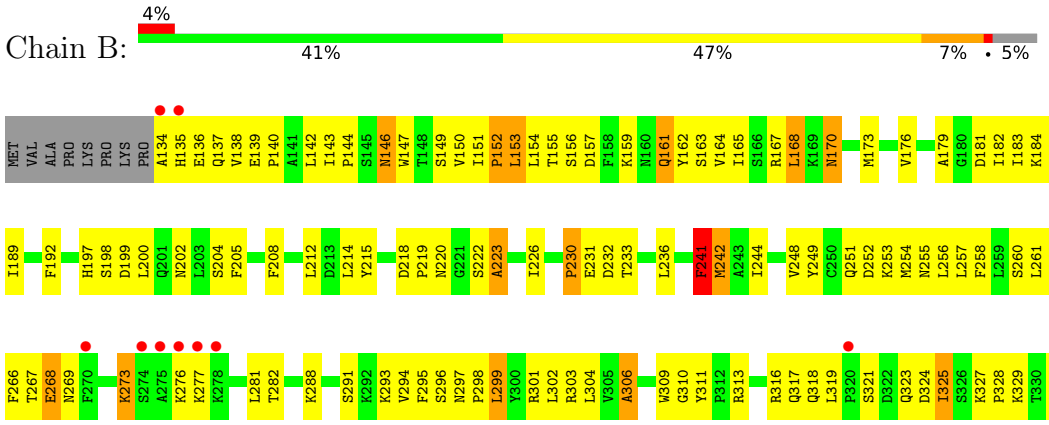
• Molecule 1: IMITATION SWITCH PROTEIN 1 (DEL_ATPASE)

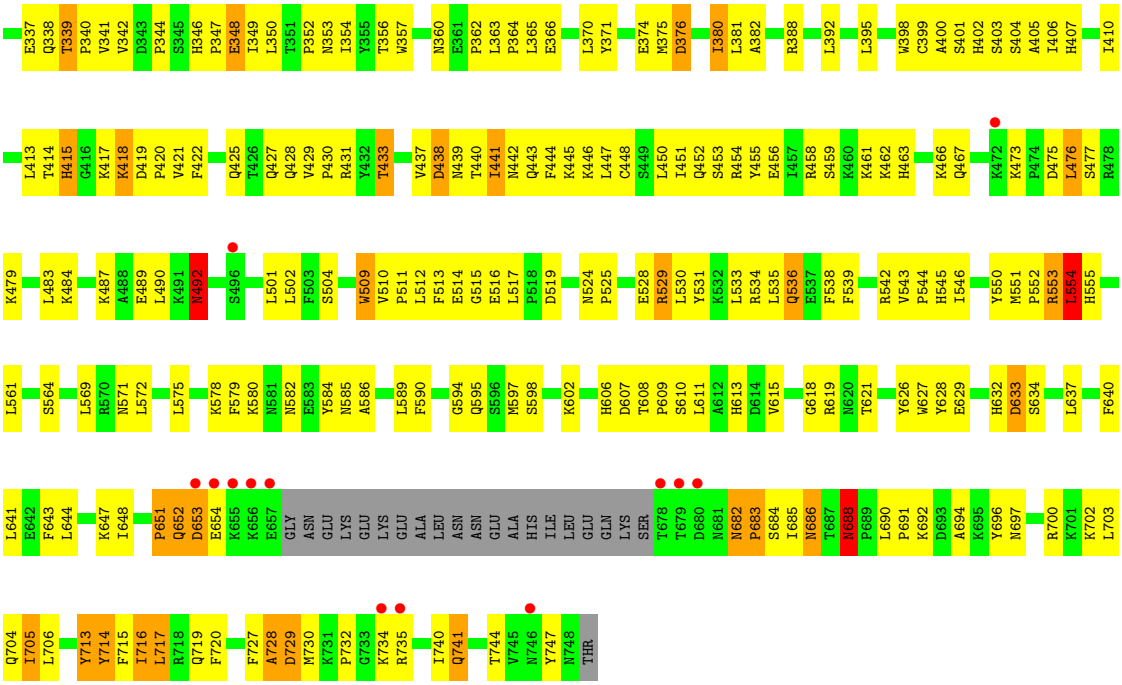
Chain A:



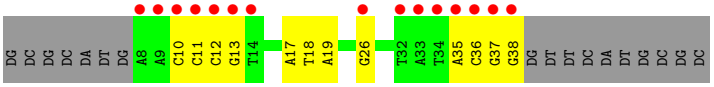
• Molecule 2: ISWI ONE COMPLEX PROTEIN 3

Chain B:

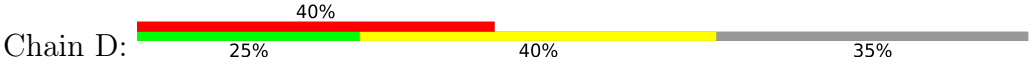


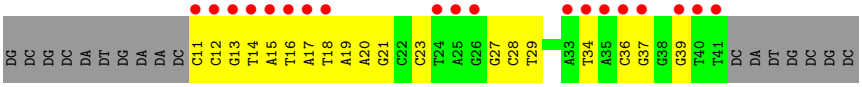


• Molecule 3: I-DNA/E-DNA

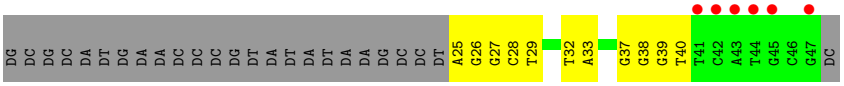


• Molecule 3: I-DNA/E-DNA





• Molecule 3: I-DNA/E-DNA



• Molecule 3: I-DNA/E-DNA

4 Data and refinement statistics (i)

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) 99.9 (29.95-3.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.61 (at 3.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.283 , 0.291 0.279 , (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)	0.30 , 104.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.25	0/2455	0.40	0/3297
2	B	0.26	0/5005	0.41	0/6769
3	C	0.47	0/712	1.00	0/1096
3	D	0.47	0/712	1.05	0/1097
3	E	0.47	0/532	1.14	0/820
3	F	0.47	0/524	1.04	0/805
All	All	0.32	0/9940	0.65	0/13884

There are no bond length outliers.

There are no bond angle outliers.

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	2404	0	2394	155	0
2	B	4882	0	4870	315	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	502	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 28.

All (502) 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
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
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:461:LYS:HZ3	2:B:463:HIS:H	1.32	0.77
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
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
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
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:982:HIS:C	1:A:984:PRO:HD3	2.12	0.69
1:A:833:PRO:HG2	1:A:858:LEU:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:682:ASN:C	2:B:684:SER:H	2.00	0.64
2:B:578:LYS:HD3	2:B:584:TYR:HE2	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:219:PRO:C	2:B:220:ASN:HD22	2.03	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
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:797:ARG:C	1:A:799:PRO:HD3	2.20	0.61
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
1:A:980:LEU:HA	1:A:982:HIS:CE1	2.36	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:993:SER:HG	1:A:996:GLU:H	1.51	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: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
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
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:157:ASP:C	2:B:159:LYS:N	2.59	0.54
2:B:403:SER:C	2:B:405:ALA:H	2.10	0.54
2:B:606:HIS:ND1	2:B:608:THR:HG23	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:447:LEU:HD23	2:B:447:LEU:C	2.28	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
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:1003:MET:HE1	2:B:619:ARG:HD2	1.89	0.53
2:B:329:LYS:HG2	2:B:357:TRP:CD1	2.44	0.53
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: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:182:ILE:HG22	2:B:186:MET:HE2	1.92	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
3:F:18:DT:H1'	3:F:19:DA:H5"	1.91	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:461:LYS:HD3	2:B:461:LYS:C	2.30	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:154:LEU:C	2:B:156:SER:H	2.12	0.52
2:B:414:THR:HG23	2:B:415:HIS:N	2.25	0.51
2:B:551:MET:HE1	2:B:717:LEU:HD11	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:403:SER:C	2:B:405:ALA:N	2.64	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
2:B:317:GLN:HB2	2:B:363:LEU:HD13	1.92	0.50
2:B:441:ILE:O	2:B:444:PHE:HB3	2.11	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:DT:H2"	3:C:19:DA:H5'	1.94	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
1:A:1036:SER:C	1:A:1037:ARG:HD2	2.32	0.48
2:B:452:GLN:HG3	2:B:487:LYS:HE2	1.94	0.48
1:A:799:PRO:O	1:A:800:LYS:HB3	2.13	0.48
2:B:375:MET:O	2:B:376:ASP:C	2.51	0.48
2:B:168:LEU:HD13	2:B:173:MET:SD	2.53	0.48
2:B:475:ASP:C	2:B:477:SER:H	2.16	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
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
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:163:SER:C	2:B:165:ILE:H	2.18	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:682:ASN:C	2:B:684:SER:N	2.66	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: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: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:157:ASP:C	2:B:159:LYS:H	2.16	0.47
2:B:713:TYR:O	2:B:714:TYR:C	2.53	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:536:GLN:NE2	2:B:550:TYR:HE2	2.12	0.47
2:B:346:HIS:O	2:B:348:GLU:N	2.48	0.47
2:B:433:THR:HG21	2:B:539:PHE:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:553:ARG:C	2:B:554:LEU:HD13	2.35	0.46
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:572:LEU:HD13	2:B:572:LEU:C	2.36	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:154:LEU:C	2:B:156:SER:N	2.70	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:1003:MET:CE	2:B:619:ARG:HD2	2.46	0.45
1:A:1036:SER:HA	2:B:400:ALA:O	2.16	0.45
1:A:807:HIS:C	1:A:809:LEU:H	2.20	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:564:SER:HB3	2:B:597:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:365:LEU:HD22	2:B:371:TYR:CE2	2.52	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: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
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:346:HIS:C	2:B:348:GLU:H	2.20	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: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
2:B:705:ILE:CG1	2:B:706:LEU:N	2.78	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
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: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
2:B:318:GLN:O	2:B:319:LEU:C	2.55	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
2:B:651:PRO:C	2:B:653:ASP:H	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
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
2:B:186:MET:HE3	2:B:552:PRO:HB3	2.01	0.43
2:B:251:GLN:O	2:B:252:ASP:C	2.55	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: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:901:LYS:C	1:A:903:GLY:H	2.21	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
2:B:652:GLN:C	2:B:654:GLU:H	2.22	0.43
1:A:815:LYS:HD3	1:A:815:LYS:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:538:PHE:HE1	2:B:553:ARG:H	1.59	0.42
2:B:433:THR:HG21	2:B:539:PHE:CD2	2.55	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: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:908:GLN:HG3	2:B:338:GLN:OE1	2.18	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:1047:ASN:O	1:A:1051:GLN:HG3	2.20	0.42
2:B:146:ASN:HD22	2:B:146:ASN:C	2.21	0.42
2:B:342:VAL:O	2:B:344:PRO:HD3	2.19	0.42
2:B:569:LEU:C	2:B:569:LEU:HD13	2.40	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: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
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
2:B:528:GLU:O	2:B:529:ARG:C	2.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1006:LYS:HZ2	2:B:619:ARG:HD3	1.84	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
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
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: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:317:GLN:O	2:B:318:GLN:C	2.58	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:265:THR:HA	2:B:403:SER:OG	2.20	0.41
2:B:428:GLN:O	2:B:535:LEU:HA	2.21	0.41
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:302:LEU:C	2:B:302:LEU:HD23	2.42	0.40
1:A:968:LEU:C	1:A:970:GLU:H	2.23	0.40
2:B:220:ASN:HD22	2:B:220:ASN:N	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:995:GLU:O	1:A:996:GLU:C	2.60	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
2:B:627:TRP:C	2:B:628:TYR:CD1	2.95	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 (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	285/374 (76%)	205 (72%)	69 (24%)	11 (4%)	3 27
2	B	591/624 (95%)	411 (70%)	138 (23%)	42 (7%)	1 14
All	All	876/998 (88%)	616 (70%)	207 (24%)	53 (6%)	1 17

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
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

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Mol	Chain	Res	Type
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 (i)

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%)	25	59
2	B	546/571 (96%)	511 (94%)	35 (6%)	17	52
All	All	810/914 (89%)	762 (94%)	48 (6%)	19	55

All (48) 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
1	A	931	TRP
1	A	949	ASN
1	A	962	GLU
1	A	964	LEU
1	A	973	ASN
1	A	980	LEU
1	A	982	HIS
1	A	1034	PHE
1	A	1061	ILE

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Mol	Chain	Res	Type
2	B	146	ASN
2	B	161	GLN
2	B	168	LEU
2	B	170	ASN
2	B	233	THR
2	B	241	PHE
2	B	255	ASN
2	B	268	GLU
2	B	273	LYS
2	B	299	LEU
2	B	309	TRP
2	B	333	PHE
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	448	CYS
2	B	455	TYR
2	B	492	ASN
2	B	509	TRP
2	B	514	GLU
2	B	536	GLN
2	B	553	ARG
2	B	554	LEU
2	B	582	ASN
2	B	652	GLN
2	B	682	ASN
2	B	688	ASN
2	B	705	ILE
2	B	713	TYR
2	B	716	ILE
2	B	717	LEU
2	B	741	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	810	GLN
1	A	863	ASN
1	A	864	ASN

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Mol	Chain	Res	Type
1	A	886	ASN
1	A	905	ASN
1	A	949	ASN
1	A	973	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	452	GLN
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	652	GLN
2	B	681	ASN
2	B	682	ASN
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 monosaccharides 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, 95^{th} 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%)	0.10	17 (5%)	22	13	86, 134, 225, 267	0
2	B	595/624 (95%)	0.02	23 (3%)	39	25	73, 120, 216, 286	0
3	C	31/48 (64%)	2.40	15 (48%)	0	0	232, 307, 423, 494	0
3	D	31/48 (64%)	2.78	19 (61%)	0	0	227, 325, 421, 433	0
3	E	23/48 (47%)	0.95	6 (26%)	0	0	118, 237, 356, 404	0
3	F	23/48 (47%)	0.91	6 (26%)	0	0	107, 239, 376, 389	0
All	All	990/1190 (83%)	0.24	86 (8%)	10	6	73, 130, 307, 494	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	40	DT	8.5
1	A	795	HIS	6.5
3	D	41	DT	6.5
3	C	37	DG	6.1
2	B	678	THR	6.0
3	C	10	DC	5.9
1	A	791	SER	5.4
3	C	38	DG	5.3
3	C	34	DT	5.0
3	D	11	DC	4.9
3	D	12	DC	4.8
3	C	33	DA	4.7
3	D	39	DG	4.6
1	A	1075	ASP	4.5
3	D	13	DG	4.4
3	D	16	DT	4.3
3	C	35	DA	4.2
3	D	34	DT	4.1
3	D	14	DT	4.1

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Mol	Chain	Res	Type	RSRZ
3	C	14	DT	3.9
1	A	789	ARG	3.9
3	F	2	DC	3.8
3	D	15	DA	3.7
3	E	44	DT	3.7
2	B	656	LYS	3.7
3	C	36	DC	3.7
1	A	796	PRO	3.7
2	B	134	ALA	3.6
3	C	11	DC	3.6
1	A	794	SER	3.5
3	E	43	DA	3.5
2	B	680	ASP	3.4
2	B	735	ARG	3.3
3	E	45	DG	3.3
2	B	746	ASN	3.3
1	A	1074	GLU	3.3
3	C	32	DT	3.3
2	B	276	LYS	3.3
3	D	36	DC	3.2
1	A	1071	MET	3.2
3	F	10	DC	3.2
2	B	657	GLU	3.2
3	C	9	DA	3.2
3	C	13	DG	3.1
1	A	1063	LEU	3.1
3	D	33	DA	3.1
2	B	653	ASP	3.1
1	A	981	LYS	3.1
1	A	793	PRO	3.0
3	D	17	DA	3.0
2	B	278	LYS	3.0
3	C	26	DG	3.0
2	B	679	THR	2.9
3	D	25	DA	2.9
1	A	790	SER	2.8
3	D	26	DG	2.8
2	B	654	GLU	2.8
2	B	274	SER	2.8
3	D	35	DA	2.8
1	A	1069	ASP	2.7
2	B	320	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	47	DG	2.6
3	E	42	DC	2.6
2	B	270	PHE	2.5
2	B	277	LYS	2.5
1	A	803	VAL	2.5
2	B	472	LYS	2.5
2	B	496	SER	2.5
3	C	8	DA	2.5
3	F	9	DA	2.5
2	B	275	ALA	2.4
3	D	37	DG	2.4
3	F	7	DG	2.4
3	C	12	DC	2.3
1	A	1067	THR	2.3
2	B	655	LYS	2.3
2	B	135	HIS	2.2
3	D	18	DT	2.2
2	B	734	LYS	2.2
3	F	3	DG	2.1
2	B	332	LEU	2.1
1	A	842	TYR	2.1
1	A	854	LYS	2.0
3	E	41	DT	2.0
3	F	8	DA	2.0
3	D	24	DT	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 monosaccharides 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.