Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 01:30 PM EDT

PDB ID	:	6O16
Title	:	Crystal structure of murine DHX37 in complex with RNA
Authors	:	Boneberg, F.; Brandmann, T.; Kobel, L.; van den Heuvel, J.; Bargsten, K.; Bammert, L.; Kutay, U.; Jinek, M.
Deposited on	:	2019-02-18
Resolution	:	2.88 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 (i) 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 (1)) were used in the production of this report:

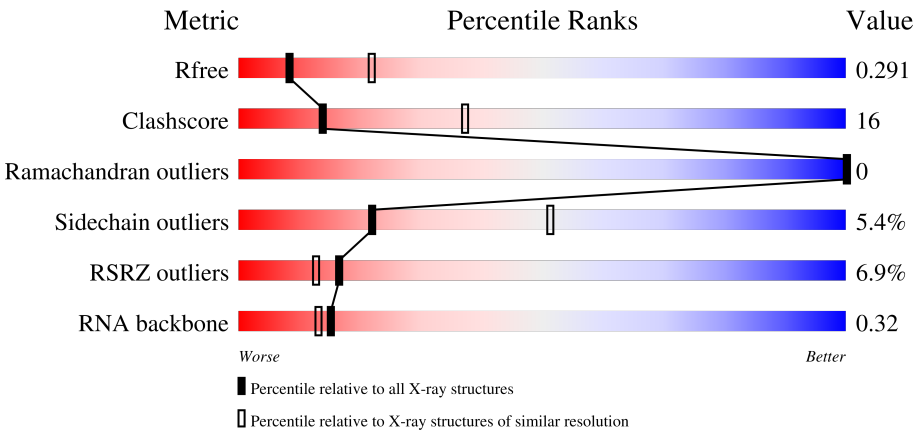
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.88 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}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)
RNA backbone	3102	1121 (3.16-2.60)

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	975	6%, 53%, 27%, •, 18%
1	B	975	5%, 54%, 26%, •, 18%
2	C	10	30%, 40%, 30%
2	D	10	30%, 50%, 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12999 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 DEAH (Asp-Glu-Ala-His) box polypeptide 37.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	798	6310	4053	1090	1129	38	0	0	0
1	B	797	6295	4050	1087	1119	39	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	SER	-	expression tag	UNP Q6NZL1
A	177	ASN	-	expression tag	UNP Q6NZL1
A	178	ALA	-	expression tag	UNP Q6NZL1
B	176	SER	-	expression tag	UNP Q6NZL1
B	177	ASN	-	expression tag	UNP Q6NZL1
B	178	ALA	-	expression tag	UNP Q6NZL1

- Molecule 2 is a RNA chain called RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

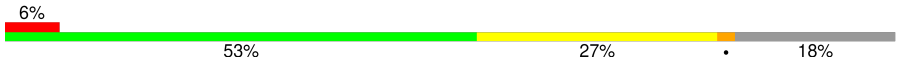
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	10	197	90	20	78	9	0	0	0
2	D	10	197	90	20	78	9	0	0	0

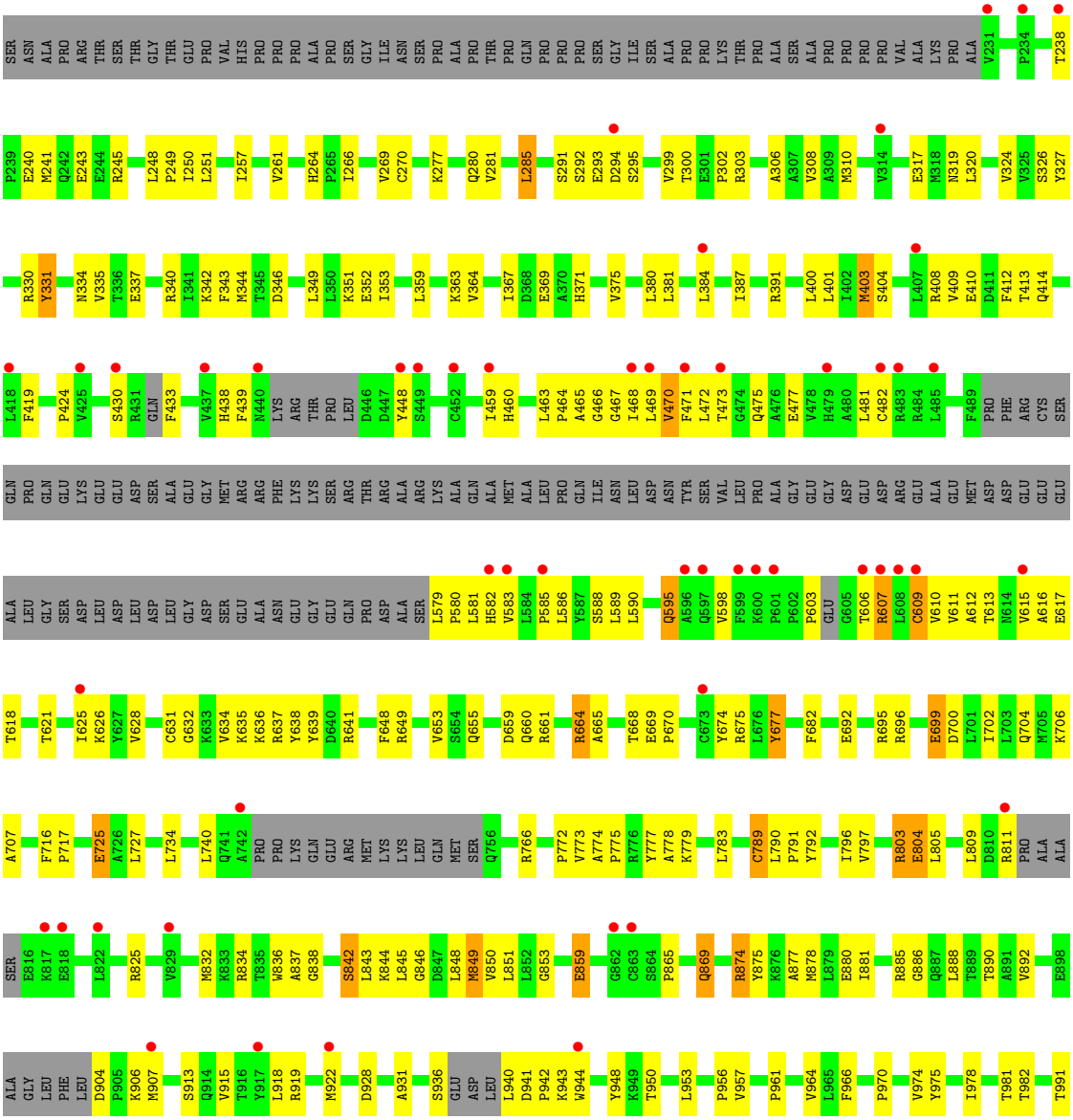
3 Residue-property plots (i)

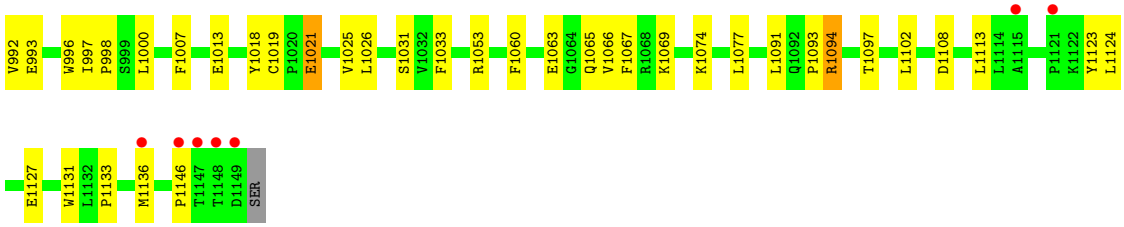
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DEAH (Asp-Glu-Ala-His) box polypeptide 37

Chain A:

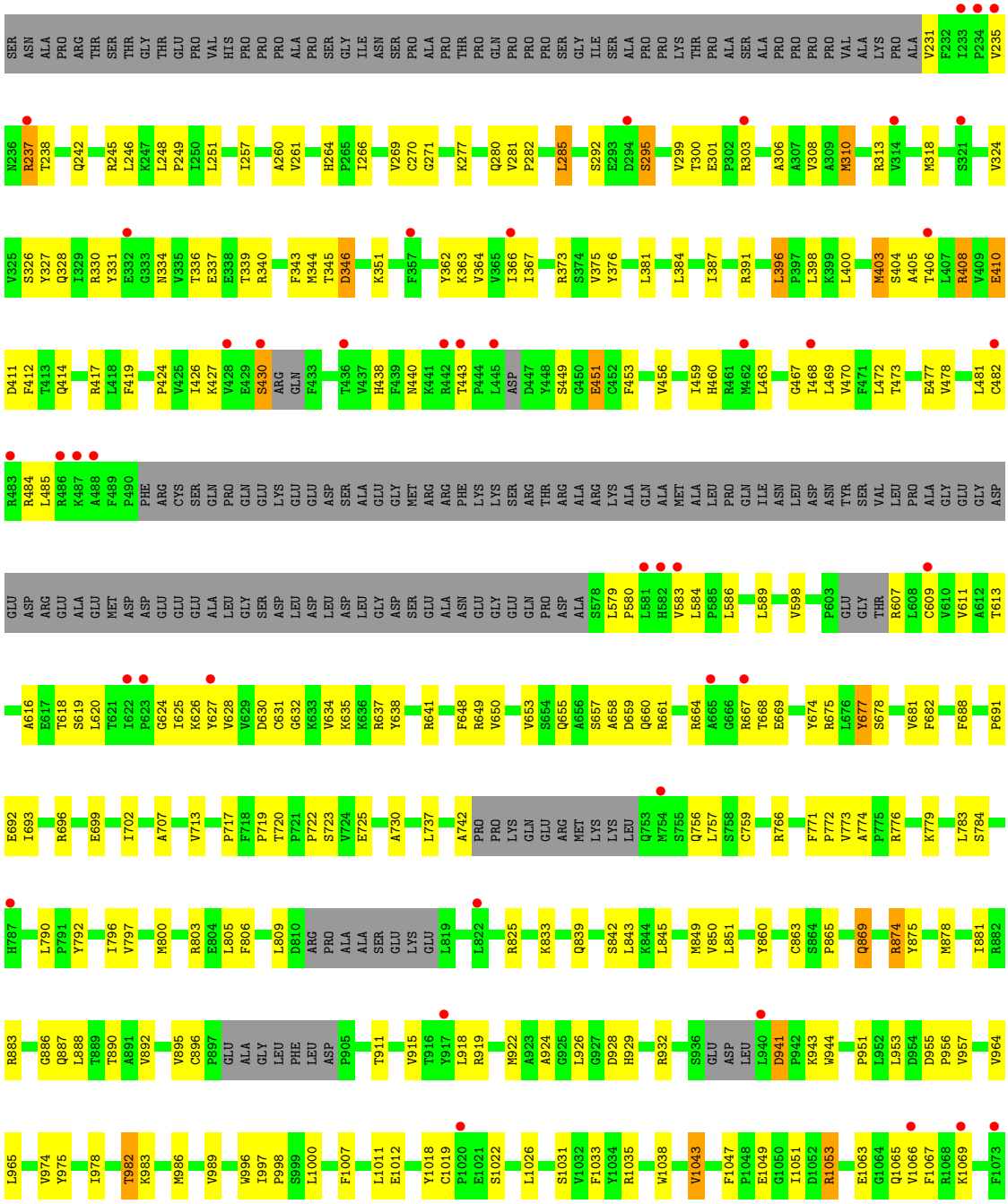


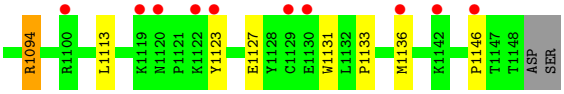




• Molecule 1: DEAH (Asp-Glu-Ala-His) box polypeptide 37

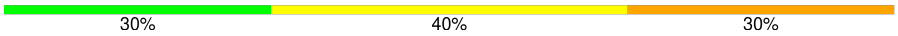
Chain B:

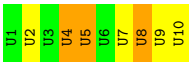




• Molecule 2: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

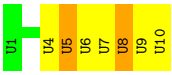
Chain C:





• Molecule 2: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.83Å 137.59Å 94.22Å 90.00° 93.34° 90.00°	Depositor
Resolution (Å)	47.03 – 2.88 47.03 – 2.88	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.03-2.88) 84.5 (47.03-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.270 , 0.295 0.270 , 0.291	Depositor DCC
R_{free} test set	2388 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	64.7	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 28.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12999	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% 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 (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	0.31	0/6451	0.49	0/8747
1	B	0.30	0/6438	0.48	0/8731
2	C	0.30	0/216	0.79	0/332
2	D	0.29	0/216	0.87	0/332
All	All	0.31	0/13321	0.50	0/18142

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 (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	6310	0	6453	211	0
1	B	6295	0	6460	201	0
2	C	197	0	102	7	0
2	D	197	0	102	6	0
All	All	12999	0	13117	413	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (413) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:VAL:HG23	1:B:653:VAL:HG22	1.48	0.95
1:A:295:SER:HB3	1:A:363:LYS:HB2	1.48	0.94
1:A:634:VAL:HG23	1:A:653:VAL:HG12	1.56	0.87
1:A:249:PRO:HG3	1:A:430:SER:HA	1.57	0.85
1:A:791:PRO:HB2	1:A:907:MET:SD	2.19	0.82
1:B:367:ILE:HD11	1:B:384:LEU:HD12	1.63	0.80
1:B:473:THR:HG22	1:B:635:LYS:HB2	1.63	0.80
1:A:621:THR:HG22	1:A:664:ARG:HH12	1.45	0.79
1:A:470:VAL:HG13	1:A:611:VAL:HA	1.65	0.78
1:B:850:VAL:HG21	1:B:964:VAL:HG21	1.65	0.78
1:A:803:ARG:NH2	2:C:5:U:O2	2.17	0.77
1:A:618:THR:HG22	1:A:660:GLN:HE22	1.49	0.76
1:A:472:LEU:HD13	1:A:477:GLU:HB3	1.66	0.76
1:B:620:LEU:O	1:B:664:ARG:NH2	2.19	0.76
1:A:655:GLN:NE2	1:A:682:PHE:O	2.19	0.75
1:A:641:ARG:HD2	1:A:725:GLU:HB2	1.68	0.75
1:B:295:SER:HB2	1:B:363:LYS:HB2	1.68	0.75
1:A:582:HIS:N	1:A:607:ARG:O	2.16	0.75
1:B:655:GLN:NE2	1:B:682:PHE:O	2.16	0.75
1:A:460:HIS:HA	1:A:607:ARG:HH21	1.52	0.74
1:A:460:HIS:NE2	1:A:580:PRO:O	2.23	0.72
1:B:998:PRO:HB2	1:B:1043:VAL:HG21	1.72	0.71
1:B:618:THR:HG22	1:B:660:GLN:HE22	1.56	0.71
1:B:825:ARG:NH2	1:B:869:GLN:OE1	2.24	0.69
1:B:440:ASN:ND2	1:B:451:GLU:OE2	2.25	0.69
1:A:367:ILE:HD11	1:A:384:LEU:HD12	1.74	0.69
1:B:472:LEU:HD13	1:B:477:GLU:HB3	1.75	0.68
1:B:271:GLY:O	1:B:277:LYS:NZ	2.19	0.68
1:B:459:ILE:HA	1:B:463:LEU:HD12	1.76	0.68
1:B:266:ILE:HG12	1:B:400:LEU:HB3	1.76	0.68
1:A:970:PRO:HG3	1:A:991:THR:HG22	1.76	0.67
1:A:319:ASN:ND2	1:B:860:TYR:O	2.26	0.67
1:A:1094:ARG:HD2	1:A:1131:TRP:CD2	2.28	0.67
1:A:375:VAL:HG23	1:A:692:GLU:HG2	1.76	0.67
1:B:845:LEU:HB3	1:B:849:MET:HG2	1.75	0.67
1:A:469:LEU:HD21	1:A:616:ALA:HB1	1.76	0.67
1:A:772:PRO:HB3	2:C:10:U:O2'	1.95	0.67
1:A:615:VAL:HG23	2:C:7:U:H5"	1.76	0.67
1:A:269:VAL:HB	1:A:403:MET:HG3	1.77	0.66
1:A:293:GLU:N	1:A:293:GLU:OE1	2.28	0.66
1:A:1133:PRO:HG2	1:A:1136:MET:HG3	1.77	0.65
1:B:809:LEU:HD13	1:B:825:ARG:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ARG:HG2	1:B:331:TYR:CD2	2.30	0.65
1:B:1019:CYS:HB2	1:B:1026:LEU:HD11	1.79	0.65
1:A:845:LEU:HB3	1:A:849:MET:HB2	1.79	0.65
1:A:919:ARG:HH22	1:A:993:GLU:HG2	1.63	0.64
1:B:641:ARG:HD2	1:B:725:GLU:HB2	1.80	0.64
1:B:1133:PRO:HG2	1:B:1136:MET:HG3	1.78	0.64
1:A:637:ARG:O	1:A:695:ARG:NH2	2.30	0.64
1:B:473:THR:HG21	1:B:650:VAL:HG22	1.80	0.64
1:B:773:VAL:HG23	1:B:888:LEU:HD21	1.79	0.64
1:B:467:GLY:HA3	1:B:625:ILE:HA	1.80	0.63
1:B:327:TYR:H	1:B:334:ASN:HB3	1.63	0.63
1:A:466:GLY:H	1:A:607:ARG:HH11	1.44	0.63
1:A:459:ILE:HG23	1:A:463:LEU:HD12	1.80	0.63
1:A:306:ALA:O	1:A:310:MET:HB2	1.99	0.63
1:A:638:TYR:CE2	1:A:649:ARG:HB2	2.34	0.62
1:B:641:ARG:NE	1:B:725:GLU:OE1	2.19	0.62
1:B:667:ARG:NH1	1:B:668:THR:OG1	2.31	0.62
1:B:1094:ARG:HD2	1:B:1131:TRP:CD2	2.34	0.62
1:A:621:THR:HG22	1:A:664:ARG:NH1	2.15	0.62
1:B:638:TYR:HE2	1:B:649:ARG:HB2	1.64	0.61
1:A:638:TYR:HE2	1:A:649:ARG:HB2	1.65	0.61
1:A:472:LEU:HD23	1:A:631:CYS:SG	2.40	0.61
1:B:408:ARG:HB2	1:B:688:PHE:CE1	2.35	0.61
1:A:277:LYS:HD2	1:A:403:MET:HG2	1.83	0.61
1:B:1063:GLU:OE1	1:B:1065:GLN:NE2	2.33	0.61
1:B:470:VAL:HG13	1:B:611:VAL:HA	1.83	0.60
1:B:586:LEU:HD13	1:B:598:VAL:HG21	1.82	0.60
1:A:337:GLU:O	1:A:340:ARG:NH2	2.33	0.60
1:B:776:ARG:NH2	1:B:928:ASP:OD2	2.34	0.60
1:B:887:GLN:NE2	2:D:10:U:O2'	2.34	0.60
1:A:327:TYR:H	1:A:334:ASN:HB3	1.66	0.60
1:A:941:ASP:OD1	1:A:942:PRO:HD2	2.01	0.60
1:A:460:HIS:CE1	1:A:580:PRO:O	2.54	0.60
1:A:773:VAL:HG23	1:A:888:LEU:HD21	1.84	0.60
1:A:586:LEU:HD22	1:A:598:VAL:HG21	1.82	0.60
1:B:619:SER:OG	2:D:8:U:OP1	2.14	0.60
1:A:464:PRO:O	1:A:607:ARG:NH1	2.35	0.59
1:A:468:ILE:HB	1:A:609:CYS:HB2	1.85	0.59
1:B:249:PRO:HG2	1:B:430:SER:HA	1.84	0.59
1:B:330:ARG:NE	1:B:887:GLN:OE1	2.32	0.59
1:B:478:VAL:HG22	1:B:611:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:TYR:O	1:B:391:ARG:NH1	2.34	0.59
1:B:336:THR:HG22	1:B:337:GLU:H	1.68	0.59
1:A:466:GLY:N	1:A:607:ARG:HH11	2.01	0.58
1:A:626:LYS:NZ	1:A:670:PRO:O	2.34	0.58
1:B:467:GLY:HA3	1:B:624:GLY:O	2.02	0.58
1:B:805:LEU:HD23	1:B:851:LEU:HD22	1.84	0.58
1:B:842:SER:HA	1:B:915:VAL:HG11	1.85	0.58
1:A:843:LEU:HD11	1:A:964:VAL:HG12	1.85	0.58
1:A:1063:GLU:OE1	1:A:1065:GLN:NE2	2.37	0.58
1:A:859:GLU:HG3	1:A:906:LYS:HD2	1.86	0.58
1:B:373:ARG:NH1	1:B:411:ASP:OD2	2.35	0.58
1:A:581:LEU:HD11	1:A:609:CYS:HB3	1.84	0.58
1:A:775:PRO:HA	1:A:778:ALA:HB3	1.86	0.58
1:A:408:ARG:HD2	1:A:410:GLU:OE2	2.04	0.58
1:B:373:ARG:NH2	1:B:719:PRO:HB2	2.19	0.58
1:B:375:VAL:HG23	1:B:692:GLU:HB3	1.84	0.58
1:B:584:LEU:HD12	1:B:598:VAL:HA	1.83	0.58
1:B:281:VAL:O	1:B:285:LEU:HD12	2.05	0.57
1:A:248:LEU:HD13	1:A:250:ILE:HG22	1.86	0.57
1:B:308:VAL:HG22	1:B:327:TYR:CD1	2.40	0.57
1:B:346:ASP:HB2	1:B:376:TYR:HB3	1.85	0.57
1:A:702:ILE:HD11	1:A:727:LEU:HD23	1.87	0.57
1:B:482:CYS:HA	1:B:583:VAL:HG11	1.85	0.57
1:A:804:GLU:O	1:A:874:ARG:NE	2.36	0.56
1:B:658:ALA:O	1:B:675:ARG:NH2	2.37	0.56
1:B:417:ARG:HG2	1:B:717:PRO:HB3	1.88	0.56
1:A:790:LEU:HD21	1:A:892:VAL:HG11	1.88	0.56
1:A:805:LEU:HD23	1:A:851:LEU:HD22	1.87	0.56
1:B:292:SER:N	1:B:295:SER:O	2.29	0.56
1:B:772:PRO:HD2	1:B:888:LEU:HD23	1.88	0.56
1:B:996:TRP:HB3	1:B:1000:LEU:HD12	1.86	0.56
1:A:245:ARG:HG2	1:A:251:LEU:HD11	1.88	0.56
1:A:261:VAL:HG22	1:A:401:LEU:HD11	1.88	0.56
1:A:865:PRO:HG3	1:A:875:TYR:CZ	2.41	0.56
1:A:460:HIS:HE2	1:A:580:PRO:HD2	1.70	0.56
1:A:881:ILE:O	1:A:885:ARG:HG3	2.06	0.56
1:B:924:ALA:HB2	1:B:1000:LEU:HD22	1.88	0.56
1:A:850:VAL:HG21	1:A:964:VAL:HG21	1.88	0.55
1:B:443:THR:HG21	1:B:681:VAL:HG21	1.87	0.55
1:A:245:ARG:O	1:A:248:LEU:HG	2.06	0.55
1:B:373:ARG:HH22	1:B:720:THR:HG23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:941:ASP:HB3	1:B:943:LYS:HG2	1.88	0.55
1:B:944:TRP:CE3	1:B:956:PRO:HB3	2.41	0.55
1:B:299:VAL:HG22	1:B:366:ILE:HB	1.88	0.55
1:B:306:ALA:O	1:B:310:MET:HB2	2.06	0.55
1:A:848:LEU:HD13	1:A:922:MET:HE3	1.88	0.55
1:B:638:TYR:CE2	1:B:649:ARG:HB2	2.40	0.55
1:A:811:ARG:NH2	2:C:4:U:O2	2.40	0.55
1:B:264:HIS:CG	1:B:424:PRO:HG3	2.41	0.55
1:B:803:ARG:O	1:B:874:ARG:NH2	2.40	0.55
1:A:772:PRO:HD2	1:A:888:LEU:HD23	1.88	0.55
1:B:653:VAL:CG1	1:B:657:SER:HB2	2.36	0.55
1:A:460:HIS:CE1	1:A:607:ARG:HE	2.25	0.54
1:A:1018:TYR:HB2	1:A:1060:PHE:CD2	2.42	0.54
1:B:586:LEU:HD21	1:B:620:LEU:HD12	1.88	0.54
1:B:1047:PHE:HB3	1:B:1053:ARG:HG3	1.89	0.54
1:A:469:LEU:HB3	1:A:628:VAL:HG12	1.90	0.54
1:A:618:THR:CG2	1:A:660:GLN:HE22	2.18	0.54
1:B:271:GLY:O	1:B:405:ALA:HA	2.06	0.54
2:C:5:U:OP2	2:C:5:U:H4'	2.08	0.54
1:A:469:LEU:O	1:A:628:VAL:HA	2.07	0.54
1:B:618:THR:HG22	1:B:660:GLN:NE2	2.23	0.54
1:B:391:ARG:HG3	1:B:396:LEU:O	2.07	0.54
1:A:617:GLU:O	1:A:660:GLN:NE2	2.41	0.54
1:B:245:ARG:HG2	1:B:251:LEU:HD11	1.90	0.54
1:A:473:THR:HG23	1:A:635:LYS:HB2	1.90	0.54
1:B:469:LEU:HB3	1:B:628:VAL:HG22	1.90	0.54
1:A:874:ARG:HH21	1:A:877:ALA:HB2	1.72	0.53
1:A:1007:PHE:CD2	1:A:1031:SER:HB3	2.43	0.53
1:B:285:LEU:HD22	1:B:364:VAL:HG21	1.90	0.53
1:B:845:LEU:HD23	1:B:849:MET:HG2	1.90	0.53
1:B:269:VAL:O	1:B:403:MET:HA	2.09	0.53
1:B:975:TYR:CE1	1:B:978:ILE:HG13	2.44	0.53
1:A:467:GLY:HA3	1:A:625:ILE:HA	1.91	0.53
1:A:632:GLY:C	1:A:653:VAL:HG13	2.28	0.53
1:B:675:ARG:HD3	1:B:677:TYR:CE2	2.44	0.53
1:A:344:MET:HE1	1:A:352:GLU:OE2	2.09	0.53
1:A:700:ASP:O	1:A:704:GLN:HG2	2.09	0.53
1:B:324:VAL:HA	1:B:339:THR:HA	1.91	0.53
1:B:1018:TYR:CZ	1:B:1066:VAL:HA	2.44	0.53
1:A:465:ALA:HA	1:A:607:ARG:HD2	1.91	0.52
1:B:773:VAL:HG21	1:B:888:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:LEU:HB3	1:A:580:PRO:HD3	1.92	0.52
1:A:330:ARG:HD3	1:A:331:TYR:CZ	2.44	0.52
1:A:238:THR:HB	1:A:241:MET:SD	2.50	0.52
1:B:473:THR:HG22	1:B:635:LYS:HE3	1.92	0.52
1:A:285:LEU:HD22	1:A:364:VAL:HG11	1.91	0.52
1:B:391:ARG:NH2	1:B:398:LEU:HB2	2.24	0.52
1:A:460:HIS:NE2	1:A:580:PRO:HD2	2.24	0.52
1:B:742:ALA:HA	1:B:759:CYS:HA	1.91	0.52
1:B:843:LEU:O	1:B:965:LEU:HD21	2.10	0.52
1:A:582:HIS:HB2	1:A:606:THR:HG22	1.91	0.51
1:A:308:VAL:HG22	1:A:327:TYR:CD1	2.45	0.51
1:B:742:ALA:HB2	1:B:759:CYS:HB3	1.91	0.51
1:B:779:LYS:O	1:B:783:LEU:HB2	2.10	0.51
1:A:330:ARG:HH21	1:A:772:PRO:HB2	1.75	0.51
1:B:630:ASP:OD2	1:B:677:TYR:OH	2.28	0.51
1:A:931:ALA:HB2	1:A:950:THR:HG22	1.92	0.51
1:A:842:SER:HA	1:A:915:VAL:HG11	1.91	0.51
1:B:707:ALA:O	1:B:766:ARG:NH1	2.42	0.51
1:B:460:HIS:ND1	1:B:607:ARG:HD3	2.26	0.51
1:B:1007:PHE:CD2	1:B:1031:SER:HB3	2.45	0.51
1:B:473:THR:CG2	1:B:635:LYS:HB2	2.38	0.51
1:B:281:VAL:HG22	1:B:282:PRO:HD3	1.92	0.51
1:B:246:LEU:HA	1:B:251:LEU:HD12	1.91	0.50
1:B:668:THR:HG22	1:B:668:THR:O	2.11	0.50
1:B:918:LEU:O	1:B:922:MET:HG2	2.10	0.50
1:A:628:VAL:HG22	1:A:665:ALA:HB2	1.92	0.50
2:D:5:U:H4'	2:D:5:U:OP1	2.10	0.50
1:A:281:VAL:O	1:A:285:LEU:HD12	2.11	0.50
1:A:943:LYS:HE2	1:A:944:TRP:HE1	1.74	0.50
1:B:346:ASP:OD1	1:B:346:ASP:N	2.45	0.50
1:B:248:LEU:CD2	1:B:280:GLN:HE21	2.25	0.50
1:B:456:VAL:HG11	1:B:485:LEU:HD11	1.94	0.50
1:A:257:ILE:O	1:A:261:VAL:HG23	2.12	0.50
1:B:929:HIS:O	1:B:974:VAL:HA	2.12	0.50
1:A:668:THR:O	1:A:669:GLU:HG3	2.12	0.50
1:B:237:ARG:HD3	1:B:242:GLN:OE1	2.11	0.50
1:B:300:THR:HA	1:B:344:MET:O	2.12	0.50
1:B:404:SER:OG	1:B:406:THR:O	2.29	0.49
1:B:579:LEU:HD12	1:B:580:PRO:HD2	1.94	0.49
1:B:583:VAL:O	1:B:584:LEU:HD23	2.11	0.49
1:B:982:THR:OG1	1:B:983:LYS:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:GLY:C	1:B:653:VAL:HG23	2.33	0.49
1:A:586:LEU:O	1:A:612:ALA:HA	2.12	0.49
1:A:269:VAL:O	1:A:403:MET:HA	2.11	0.49
1:A:598:VAL:HG13	1:A:610:VAL:HG21	1.93	0.49
1:B:1019:CYS:HB3	1:B:1022:SER:HB3	1.94	0.49
1:A:266:ILE:HD13	1:A:419:PHE:CE1	2.48	0.49
1:A:943:LYS:HE2	1:A:944:TRP:NE1	2.28	0.49
1:B:438:HIS:HB2	1:B:674:TYR:CD1	2.48	0.49
1:B:634:VAL:HG22	1:B:661:ARG:NH2	2.28	0.49
1:A:369:GLU:HA	1:A:371:HIS:CE1	2.48	0.49
1:A:381:LEU:HD13	1:A:412:PHE:CE1	2.48	0.49
1:B:453:PHE:HE1	1:B:485:LEU:HD23	1.78	0.49
1:A:886:GLY:O	1:A:890:THR:HG23	2.12	0.48
1:A:292:SER:N	1:A:295:SER:O	2.47	0.48
1:A:931:ALA:HB1	1:A:948:TYR:HB3	1.96	0.48
1:B:408:ARG:NE	1:B:408:ARG:O	2.46	0.48
1:A:777:TYR:HB3	1:A:797:VAL:HG13	1.95	0.48
1:A:789:CYS:HA	1:A:792:TYR:CD2	2.47	0.48
1:A:961:PRO:HA	1:A:966:PHE:CD1	2.49	0.48
1:A:1018:TYR:CZ	1:A:1066:VAL:HA	2.48	0.48
1:B:336:THR:HG22	1:B:337:GLU:N	2.27	0.48
1:B:943:LYS:HG3	1:B:944:TRP:CD1	2.47	0.48
1:A:349:LEU:HD11	1:A:359:LEU:HD21	1.94	0.48
1:A:433:PHE:CD2	1:A:668:THR:HA	2.48	0.48
1:A:792:TYR:O	1:A:796:ILE:HG13	2.13	0.48
1:B:951:PRO:HB3	1:B:1035:ARG:HB3	1.95	0.48
1:A:603:PRO:O	1:A:606:THR:HB	2.14	0.48
1:B:699:GLU:HA	1:B:730:ALA:HB1	1.96	0.48
1:A:1025:VAL:HG13	1:A:1060:PHE:HE2	1.79	0.48
1:A:1067:PHE:HE2	1:A:1113:LEU:HD23	1.78	0.48
1:A:1019:CYS:HB2	1:A:1026:LEU:HD11	1.95	0.48
1:B:589:LEU:HD21	1:B:803:ARG:CZ	2.44	0.48
1:A:773:VAL:HG12	1:A:774:ALA:N	2.28	0.47
1:B:235:VAL:HG11	1:B:237:ARG:CZ	2.44	0.47
1:B:285:LEU:HD13	1:B:366:ILE:HD11	1.95	0.47
1:B:886:GLY:O	1:B:890:THR:HG23	2.14	0.47
1:A:384:LEU:HD13	1:A:400:LEU:HD13	1.96	0.47
1:A:974:VAL:HG13	1:A:992:VAL:HG21	1.97	0.47
1:A:636:LYS:HB3	1:A:695:ARG:NH2	2.29	0.47
1:A:874:ARG:O	1:A:878:MET:HG2	2.14	0.47
1:A:293:GLU:CD	1:A:294:ASP:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:ARG:NH1	1:A:991:THR:O	2.46	0.47
1:A:928:ASP:OD1	1:A:928:ASP:N	2.46	0.47
1:A:953:LEU:HD11	1:A:957:VAL:CG2	2.45	0.47
1:B:308:VAL:HG13	1:B:327:TYR:CE2	2.50	0.47
1:A:320:LEU:HD13	1:A:324:VAL:HG11	1.97	0.47
1:B:626:LYS:HD2	1:B:669:GLU:OE1	2.15	0.47
1:B:384:LEU:HD23	1:B:387:ILE:HD12	1.96	0.47
1:B:478:VAL:HG13	1:B:611:VAL:HB	1.96	0.47
1:A:299:VAL:O	1:A:344:MET:HG2	2.14	0.46
1:A:351:LYS:HA	1:A:351:LYS:HD3	1.77	0.46
1:B:911:THR:O	1:B:915:VAL:HG23	2.15	0.46
1:B:928:ASP:OD1	1:B:928:ASP:N	2.46	0.46
1:B:1067:PHE:HE2	1:B:1113:LEU:HD23	1.80	0.46
1:A:482:CYS:SG	1:A:583:VAL:HG12	2.55	0.46
1:A:845:LEU:HD13	1:A:919:ARG:HG2	1.96	0.46
1:B:328:GLN:O	1:B:344:MET:HA	2.15	0.46
1:A:264:HIS:CG	1:A:424:PRO:HG3	2.50	0.46
1:B:257:ILE:O	1:B:261:VAL:HG23	2.15	0.46
1:B:641:ARG:HD3	1:B:723:SER:OG	2.16	0.46
1:A:270:CYS:HA	1:A:404:SER:O	2.15	0.46
1:A:699:GLU:H	1:A:699:GLU:HG3	1.33	0.46
1:A:582:HIS:N	1:A:606:THR:HG22	2.30	0.46
1:B:443:THR:HG22	1:B:678:SER:N	2.31	0.46
1:B:459:ILE:O	1:B:463:LEU:HB2	2.16	0.46
1:B:975:TYR:CD1	1:B:978:ILE:HG13	2.49	0.46
1:A:943:LYS:HG3	1:A:944:TRP:CD1	2.50	0.46
1:B:460:HIS:HA	1:B:607:ARG:NH2	2.31	0.46
1:A:975:TYR:CE1	1:A:978:ILE:HG13	2.51	0.46
1:B:330:ARG:HH21	1:B:772:PRO:HB2	1.80	0.46
1:A:809:LEU:HD22	1:A:825:ARG:HG2	1.97	0.46
1:A:838:GLY:H	1:A:842:SER:HG	1.62	0.46
1:B:257:ILE:HA	1:B:426:ILE:HD13	1.98	0.46
1:A:837:ALA:HB2	1:A:850:VAL:HG22	1.98	0.45
1:A:944:TRP:CE3	1:A:956:PRO:HB3	2.51	0.45
1:B:408:ARG:HB2	1:B:688:PHE:CZ	2.51	0.45
1:B:453:PHE:HB2	1:B:481:LEU:HD11	1.98	0.45
1:A:702:ILE:O	1:A:706:LYS:HG2	2.16	0.45
1:A:993:GLU:HB2	1:A:996:TRP:CE2	2.51	0.45
1:A:473:THR:HG22	1:A:635:LYS:HE3	1.99	0.45
1:A:637:ARG:HD2	1:A:648:PHE:CZ	2.51	0.45
1:A:918:LEU:O	1:A:922:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:HD23	1:A:387:ILE:HD12	1.97	0.45
1:A:613:THR:OG1	2:C:7:U:OP1	2.27	0.45
1:B:635:LYS:O	2:D:6:U:H1'	2.16	0.45
1:B:953:LEU:HD11	1:B:957:VAL:CG2	2.46	0.45
1:A:996:TRP:HB3	1:A:1000:LEU:HD12	1.98	0.45
1:B:331:TYR:CZ	1:B:883:ARG:HD2	2.52	0.45
1:A:310:MET:HB3	1:A:343:PHE:CE2	2.51	0.45
1:B:237:ARG:NH1	1:B:245:ARG:HH12	2.15	0.45
1:B:659:ASP:HA	1:B:675:ARG:HH22	1.81	0.45
1:A:981:THR:OG1	1:A:982:THR:N	2.49	0.45
1:A:482:CYS:SG	1:A:585:PRO:HB3	2.56	0.45
1:A:844:LYS:HB3	1:A:991:THR:OG1	2.17	0.45
1:B:337:GLU:O	1:B:340:ARG:NH2	2.46	0.45
1:B:301:GLU:O	1:B:345:THR:HG23	2.17	0.44
1:B:978:ILE:HG12	1:B:986:MET:HB3	1.99	0.44
1:A:846:GLY:O	1:A:850:VAL:HG23	2.18	0.44
1:B:757:LEU:HD23	1:B:757:LEU:HA	1.53	0.44
1:B:843:LEU:HD11	1:B:964:VAL:HG12	1.99	0.44
1:B:391:ARG:HG2	1:B:398:LEU:HB2	1.98	0.44
1:B:410:GLU:O	1:B:414:GLN:HB2	2.17	0.44
1:A:280:GLN:NE2	1:A:317:GLU:OE1	2.50	0.44
1:B:270:CYS:HA	1:B:404:SER:O	2.17	0.44
1:B:303:ARG:NH2	1:B:618:THR:O	2.48	0.44
1:A:838:GLY:N	1:A:842:SER:OG	2.51	0.44
1:B:384:LEU:HD23	1:B:384:LEU:HA	1.67	0.44
1:A:471:PHE:CG	1:A:661:ARG:HD3	2.52	0.44
1:B:463:LEU:HD13	1:B:627:TYR:HE2	1.82	0.44
1:B:468:ILE:HB	1:B:609:CYS:HA	1.99	0.44
1:A:586:LEU:HD12	1:A:586:LEU:HA	1.65	0.44
1:A:292:SER:HB3	1:A:293:GLU:OE1	2.18	0.44
1:A:409:VAL:O	1:A:413:THR:HG22	2.17	0.43
1:A:825:ARG:NH2	1:A:869:GLN:OE1	2.51	0.43
1:A:1102:LEU:HD21	1:A:1124:LEU:HD11	1.99	0.43
1:B:266:ILE:HD13	1:B:419:PHE:CE1	2.53	0.43
1:B:637:ARG:HD2	1:B:648:PHE:CZ	2.53	0.43
1:B:773:VAL:HG12	1:B:774:ALA:N	2.33	0.43
1:A:874:ARG:NH2	1:A:877:ALA:HB2	2.33	0.43
1:B:285:LEU:HD22	1:B:364:VAL:HG11	2.00	0.43
1:A:326:SER:OG	1:A:335:VAL:HG12	2.18	0.43
1:A:438:HIS:HB2	1:A:674:TYR:HD1	1.83	0.43
1:A:936:SER:HA	1:A:940:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:ILE:HB	1:A:998:PRO:HD3	2.00	0.43
1:B:408:ARG:NH2	1:B:412:PHE:CE2	2.87	0.43
1:A:261:VAL:CG2	1:A:401:LEU:HD11	2.49	0.43
1:A:590:LEU:O	1:A:595:GLN:NE2	2.51	0.43
1:A:659:ASP:HA	1:A:675:ARG:HH22	1.84	0.43
1:B:796:ILE:HG22	1:B:800:MET:HE2	2.00	0.43
1:B:932:ARG:CZ	1:B:1038:TRP:CD1	3.02	0.43
1:B:1127:GLU:N	1:B:1127:GLU:OE1	2.48	0.43
1:B:806:PHE:CD1	1:B:833:LYS:HE3	2.54	0.43
1:A:616:ALA:O	1:A:664:ARG:HD2	2.19	0.43
1:B:303:ARG:CZ	1:B:619:SER:HA	2.49	0.43
1:B:691:PRO:HG2	1:B:720:THR:HG21	2.01	0.43
1:A:579:LEU:CB	1:A:580:PRO:HD3	2.49	0.43
1:B:790:LEU:HD21	1:B:892:VAL:HG11	2.00	0.43
1:B:792:TYR:O	1:B:796:ILE:HG13	2.19	0.43
1:A:1021:GLU:N	1:A:1021:GLU:CD	2.72	0.42
1:B:997:ILE:HB	1:B:998:PRO:HD3	2.01	0.42
1:A:240:GLU:O	1:A:243:GLU:HG2	2.19	0.42
1:A:637:ARG:NH2	1:A:639:TYR:OH	2.51	0.42
1:B:613:THR:OG1	2:D:7:U:OP1	2.22	0.42
1:A:291:SER:OG	1:A:340:ARG:HB3	2.19	0.42
1:B:260:ALA:HB3	1:B:426:ILE:HD11	2.01	0.42
1:A:241:MET:H	1:A:241:MET:HG2	1.59	0.42
1:A:248:LEU:HD21	1:A:280:GLN:NE2	2.34	0.42
1:A:675:ARG:HB3	1:A:677:TYR:CZ	2.55	0.42
1:A:300:THR:OG1	1:A:367:ILE:HA	2.19	0.42
1:A:1069:LYS:HD2	1:A:1146:PRO:HA	2.02	0.42
1:B:776:ARG:HD3	1:B:926:LEU:HD23	2.01	0.42
1:B:797:VAL:HA	1:B:800:MET:HE3	2.01	0.42
1:A:707:ALA:O	1:A:766:ARG:NH1	2.53	0.42
1:A:1074:LYS:HA	1:A:1077:LEU:HD13	2.01	0.42
1:B:865:PRO:HG3	1:B:875:TYR:CZ	2.55	0.42
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.91	0.42
1:B:257:ILE:HG12	1:B:426:ILE:HG21	2.01	0.42
1:B:895:VAL:HG12	1:B:896:CYS:SG	2.59	0.42
1:B:1069:LYS:HD2	1:B:1146:PRO:HA	2.02	0.42
1:A:832:MET:HG3	1:A:836:TRP:CZ2	2.55	0.42
1:A:948:TYR:N	1:A:957:VAL:O	2.45	0.42
1:A:1091:LEU:HD23	1:A:1091:LEU:HA	1.77	0.42
1:A:1094:ARG:HD3	1:A:1131:TRP:HA	2.02	0.42
1:A:248:LEU:HD13	1:A:250:ILE:CG2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:PRO:O	1:A:1097:THR:HG23	2.20	0.41
1:B:310:MET:HB3	1:B:343:PHE:CE2	2.55	0.41
1:B:469:LEU:HB2	1:B:625:ILE:HG21	2.00	0.41
1:B:485:LEU:HD23	1:B:485:LEU:HA	1.87	0.41
1:B:648:PHE:HE2	2:D:6:U:C5	2.37	0.41
1:A:468:ILE:O	1:A:609:CYS:HA	2.20	0.41
1:B:693:ILE:HG12	1:B:722:PRO:HB3	2.02	0.41
1:A:439:PHE:HE2	1:A:682:PHE:HB2	1.85	0.41
1:B:839:GLN:HA	1:B:843:LEU:HB2	2.02	0.41
1:A:326:SER:HB2	1:A:334:ASN:HB3	2.02	0.41
1:B:330:ARG:HG3	1:B:887:GLN:NE2	2.36	0.41
1:A:588:SER:OG	2:C:8:U:OP2	2.26	0.41
1:A:779:LYS:O	1:A:783:LEU:HB2	2.21	0.41
1:A:834:ARG:O	1:A:837:ALA:O	2.39	0.41
1:B:381:LEU:HD13	1:B:412:PHE:CE1	2.55	0.41
1:B:845:LEU:HD13	1:B:919:ARG:HG2	2.02	0.41
1:B:869:GLN:HE21	1:B:869:GLN:HB3	1.71	0.41
1:B:878:MET:SD	1:B:881:ILE:HD12	2.60	0.41
1:A:327:TYR:HA	1:A:343:PHE:O	2.21	0.41
1:B:800:MET:HE3	1:B:800:MET:HB2	1.90	0.41
1:A:349:LEU:O	1:A:353:ILE:HG13	2.21	0.41
1:A:473:THR:CG2	1:A:635:LYS:HB2	2.48	0.41
1:B:351:LYS:HD3	1:B:351:LYS:HA	1.96	0.41
1:A:342:LYS:HE2	1:A:344:MET:HE3	2.02	0.41
1:A:359:LEU:O	1:A:391:ARG:NH2	2.54	0.41
1:A:1108:ASP:OD1	1:A:1108:ASP:N	2.54	0.41
1:A:1127:GLU:OE1	1:A:1127:GLU:N	2.53	0.41
1:B:737:LEU:O	1:B:779:LYS:HE2	2.21	0.41
1:A:481:LEU:HB3	1:A:611:VAL:HG11	2.04	0.40
1:A:716:PHE:CD1	1:A:717:PRO:HD2	2.56	0.40
1:A:734:LEU:HB3	1:A:740:LEU:HG	2.03	0.40
1:A:836:TRP:HB3	1:A:853:GLY:HA3	2.02	0.40
1:B:771:PHE:HA	1:B:772:PRO:HD3	1.88	0.40
1:A:659:ASP:HA	1:A:675:ARG:NH2	2.36	0.40
1:B:410:GLU:H	1:B:410:GLU:HG2	1.43	0.40
1:A:302:PRO:HB2	1:A:303:ARG:NH1	2.36	0.40
1:A:472:LEU:HD23	1:A:631:CYS:HG	1.85	0.40
1:A:472:LEU:HA	1:A:631:CYS:SG	2.61	0.40
1:B:292:SER:HB3	1:B:295:SER:OG	2.22	0.40
1:B:237:ARG:HH11	1:B:245:ARG:HH12	1.69	0.40
1:B:616:ALA:O	1:B:664:ARG:NE	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:LEU:O	1:B:953:LEU:HD12	2.22	0.40
1:B:702:ILE:HD13	1:B:713:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	780/975 (80%)	758 (97%)	22 (3%)	0	100	100
1	B	779/975 (80%)	751 (96%)	28 (4%)	0	100	100
All	All	1559/1950 (80%)	1509 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	690/836 (82%)	656 (95%)	34 (5%)	25	55
1	B	690/836 (82%)	650 (94%)	40 (6%)	20	48
All	All	1380/1672 (82%)	1306 (95%)	74 (5%)	22	51

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	LEU
1	A	331	TYR
1	A	346	ASP
1	A	403	MET
1	A	414	GLN
1	A	448	TYR
1	A	470	VAL
1	A	475	GLN
1	A	589	LEU
1	A	595	GLN
1	A	607	ARG
1	A	609	CYS
1	A	664	ARG
1	A	677	TYR
1	A	696	ARG
1	A	699	GLU
1	A	725	GLU
1	A	789	CYS
1	A	803	ARG
1	A	804	GLU
1	A	842	SER
1	A	849	MET
1	A	859	GLU
1	A	869	GLN
1	A	874	ARG
1	A	880	GLU
1	A	904	ASP
1	A	913	SER
1	A	1013	GLU
1	A	1021	GLU
1	A	1033	PHE
1	A	1053	ARG
1	A	1094	ARG
1	A	1123	TYR
1	B	231	VAL
1	B	237	ARG
1	B	238	THR
1	B	285	LEU
1	B	295	SER
1	B	310	MET
1	B	313	ARG
1	B	318	MET
1	B	326	SER

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Mol	Chain	Res	Type
1	B	346	ASP
1	B	396	LEU
1	B	403	MET
1	B	408	ARG
1	B	410	GLU
1	B	427	LYS
1	B	430	SER
1	B	449	SER
1	B	451	GLU
1	B	484	ARG
1	B	631	CYS
1	B	677	TYR
1	B	696	ARG
1	B	756	GLN
1	B	784	SER
1	B	863	CYS
1	B	869	GLN
1	B	874	ARG
1	B	941	ASP
1	B	955	ASP
1	B	982	THR
1	B	989	VAL
1	B	1011	LEU
1	B	1012	GLU
1	B	1033	PHE
1	B	1043	VAL
1	B	1049	GLU
1	B	1051	ILE
1	B	1053	ARG
1	B	1094	ARG
1	B	1123	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	438	HIS
1	A	440	ASN
1	A	660	GLN
1	B	280	GLN
1	B	660	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	9/10 (90%)	5 (55%)	0
2	D	9/10 (90%)	3 (33%)	1 (11%)
All	All	18/20 (90%)	8 (44%)	1 (5%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	U
2	C	4	U
2	C	5	U
2	C	8	U
2	C	9	U
2	D	5	U
2	D	8	U
2	D	9	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	4	U

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 (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	798/975 (81%)	0.48	58 (7%)	15	11	30, 60, 101, 144	0
1	B	797/975 (81%)	0.46	53 (6%)	18	14	36, 63, 100, 132	0
2	C	10/10 (100%)	0.28	0	100	100	49, 57, 93, 100	0
2	D	10/10 (100%)	0.34	0	100	100	54, 66, 83, 87	0
All	All	1615/1970 (81%)	0.47	111 (6%)	16	13	30, 61, 100, 144	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	VAL	7.0
1	B	483	ARG	6.8
1	B	1073	PHE	5.7
1	A	294	ASP	5.2
1	B	667	ARG	4.6
1	A	609	CYS	4.5
1	A	817	LYS	4.4
1	A	452	CYS	4.3
1	A	583	VAL	4.3
1	B	609	CYS	4.1
1	B	1119	LYS	4.1
1	B	430	SER	4.0
1	A	407	LEU	4.0
1	B	482	CYS	4.0
1	A	601	PRO	3.9
1	B	445	LEU	3.9
1	A	468	ILE	3.8
1	B	487	LYS	3.8
1	A	596	ALA	3.7
1	B	623	PRO	3.7
1	B	581	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	459	ILE	3.5
1	B	582	HIS	3.5
1	A	862	GLY	3.4
1	B	622	ILE	3.4
1	A	811	ARG	3.3
1	B	486	ARG	3.3
1	B	468	ILE	3.2
1	A	599	PHE	3.2
1	B	665	ALA	3.2
1	B	627	TYR	3.1
1	B	822	LEU	3.1
1	A	907	MET	3.1
1	B	303	ARG	3.0
1	A	1149	ASP	3.0
1	A	485	LEU	3.0
1	B	488	ALA	2.9
1	A	818	GLU	2.9
1	B	406	THR	2.9
1	A	430	SER	2.9
1	B	583	VAL	2.9
1	B	357	PHE	2.8
1	A	449	SER	2.8
1	B	366	ILE	2.8
1	A	608	LEU	2.8
1	A	944	TRP	2.8
1	B	1142	LYS	2.7
1	A	234	PRO	2.7
1	A	582	HIS	2.7
1	B	442	ARG	2.7
1	A	606	THR	2.7
1	A	625	ILE	2.7
1	A	469	LEU	2.6
1	B	294	ASP	2.6
1	B	332	GLU	2.6
1	A	597	GLN	2.6
1	B	1136	MET	2.6
1	B	235	VAL	2.6
1	A	600	LYS	2.6
1	B	1066	VAL	2.6
1	B	1122	LYS	2.5
1	B	314	VAL	2.5
1	A	607	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	940	LEU	2.5
1	A	238	THR	2.5
1	B	1020	PRO	2.5
1	B	436	THR	2.4
1	B	1146	PRO	2.4
1	B	321	SER	2.4
1	B	1069	LYS	2.4
1	A	1148	THR	2.4
1	B	1120	ASN	2.4
1	B	234	PRO	2.4
1	A	863	CYS	2.4
1	A	585	PRO	2.3
1	A	473	THR	2.3
1	B	462	MET	2.3
1	A	384	LEU	2.3
1	A	440	ASN	2.3
1	A	1121	PRO	2.3
1	A	314	VAL	2.3
1	B	754	MET	2.3
1	B	1123	TYR	2.3
1	A	471	PHE	2.3
1	B	233	ILE	2.2
1	B	443	THR	2.2
1	A	448	TYR	2.2
1	A	822	LEU	2.2
1	B	1129	CYS	2.2
1	A	829	VAL	2.2
1	B	1100	ARG	2.1
1	A	479	HIS	2.1
1	A	673	CYS	2.1
1	A	483	ARG	2.1
1	A	742	ALA	2.1
1	A	482	CYS	2.1
1	B	917	TYR	2.1
1	A	425	VAL	2.1
1	B	428	VAL	2.1
1	A	1147	THR	2.1
1	A	418	LEU	2.0
1	B	237	ARG	2.0
1	A	615	VAL	2.0
1	A	917	TYR	2.0
1	A	1115	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	437	VAL	2.0
1	A	922	MET	2.0
1	A	1146	PRO	2.0
1	B	787	HIS	2.0
1	B	1130	GLU	2.0
1	A	1136	MET	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.