



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:21 PM UTC

PDB ID : 6O16 / pdb_00006o16
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 ⓘ 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

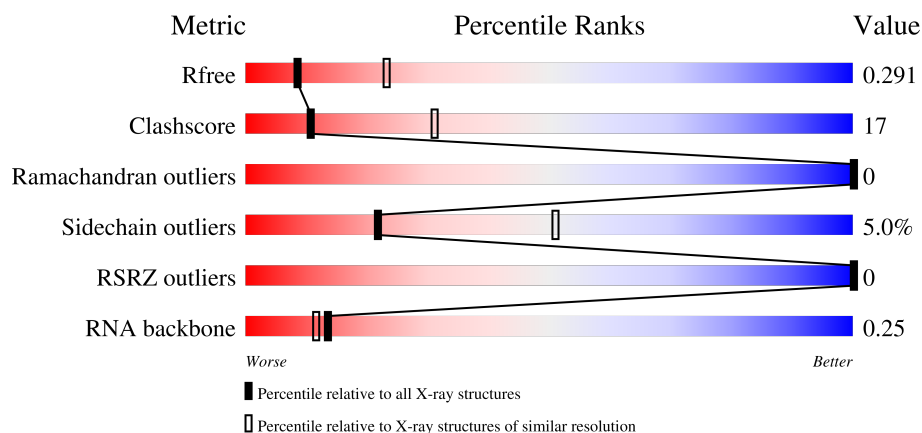
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)
RNA backbone	3983	1174 (3.10-2.66)

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	975	
1	B	975	
2	C	10	
2	D	10	

2 Entry composition

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
1	A	798	Total	C	N	O	S	0	0	0
			6310	4053	1090	1129	38			
1	B	797	Total	C	N	O	S	0	0	0
			6295	4050	1087	1119	39			

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

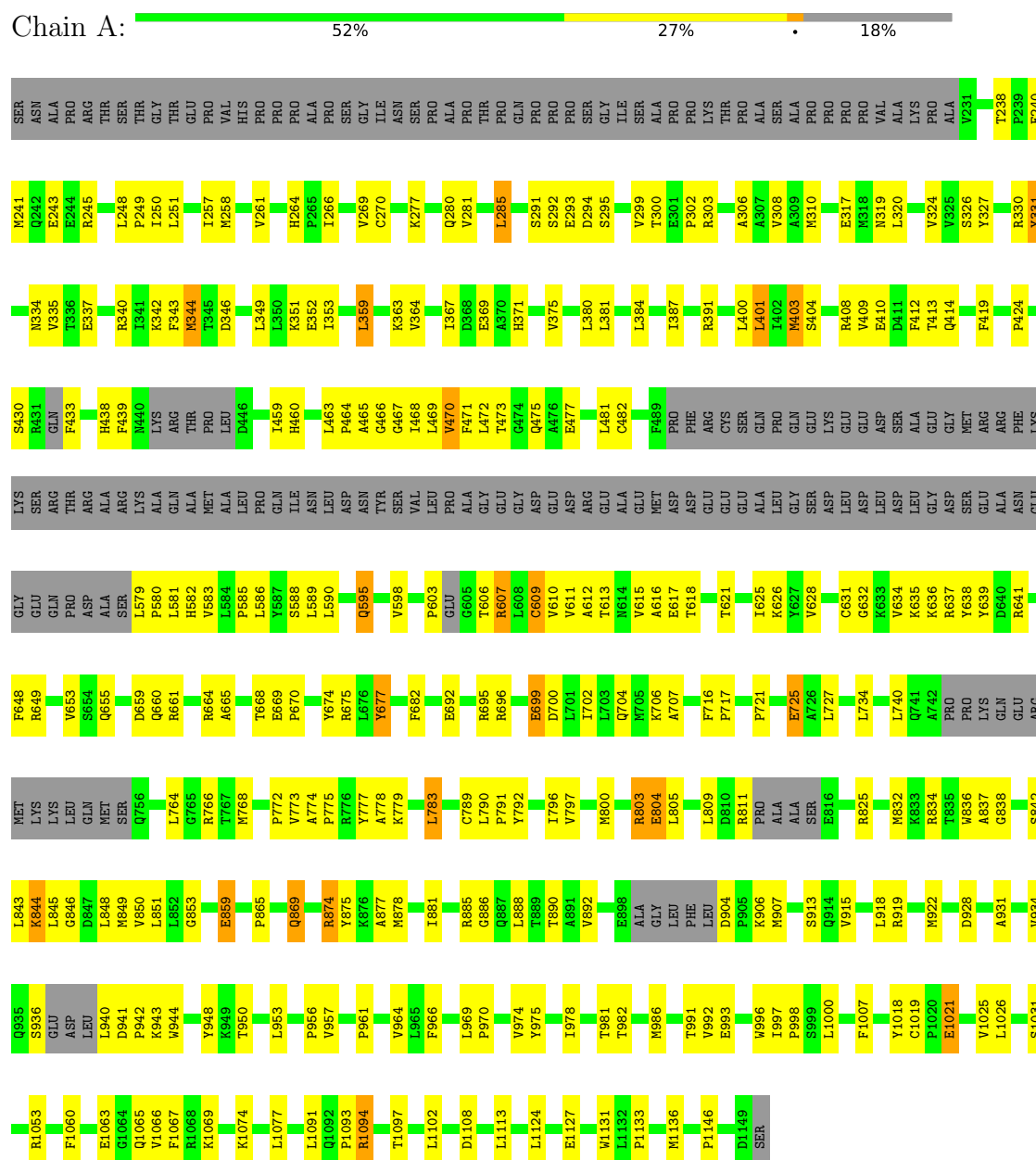
- Molecule 2 is a RNA chain called RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

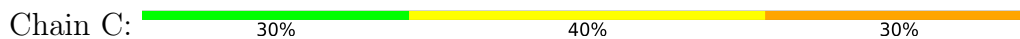
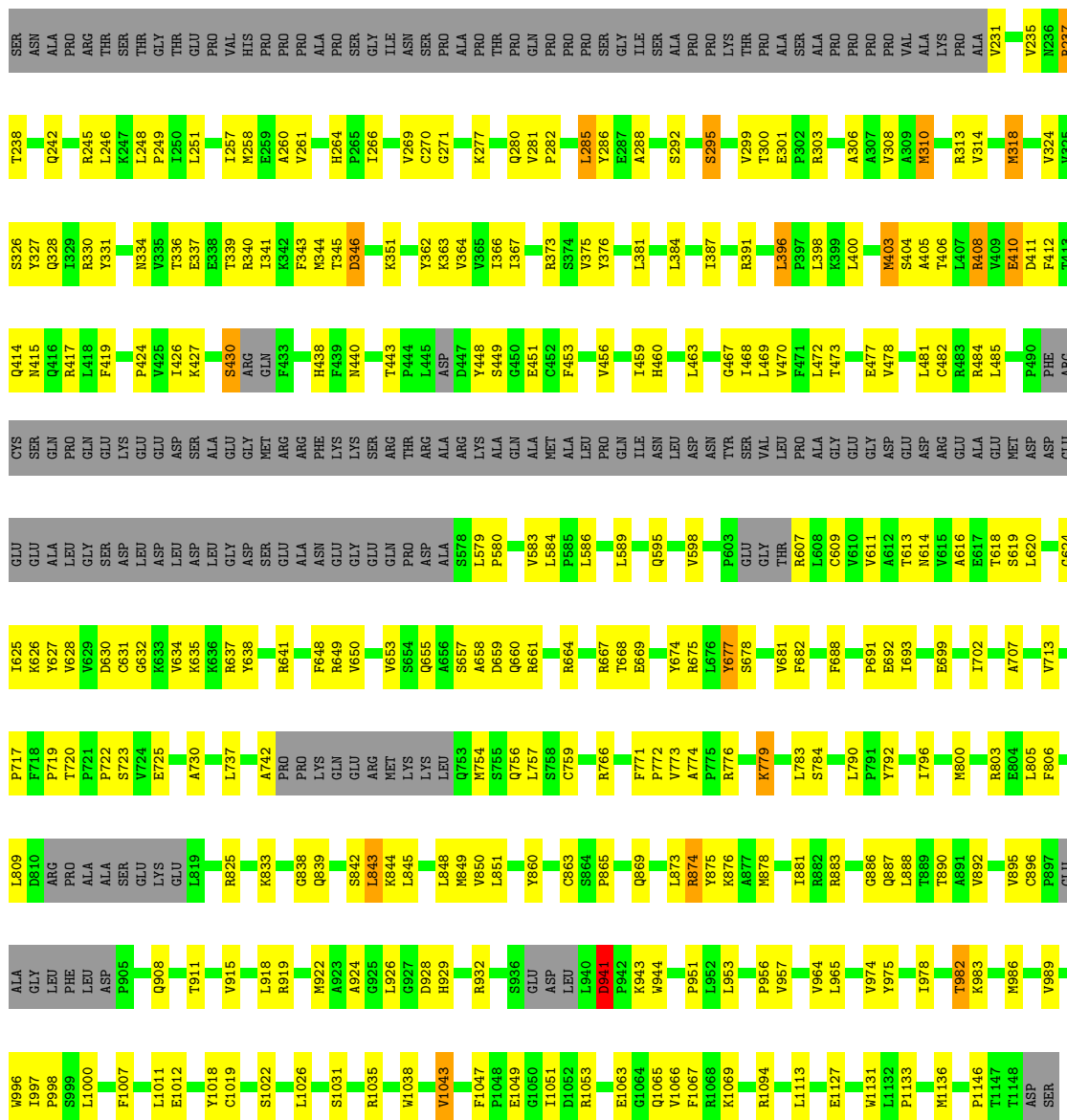
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			197	90	20	78	9			
2	D	10	Total	C	N	O	P	0	0	0
			197	90	20	78	9			

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







4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

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	0.24	2/6451 (0.0%)	0.46	1/8747 (0.0%)
1	B	0.22	0/6438	0.45	1/8731 (0.0%)
2	C	0.21	0/216	0.45	0/332
2	D	0.17	0/216	0.57	0/332
All	All	0.22	2/13321 (0.0%)	0.46	2/18142 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	969	LEU	C-O	5.66	1.26	1.23
1	A	721	PRO	CA-C	-5.09	1.48	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	941	ASP	N-CA-C	-8.20	100.78	108.07
1	A	721	PRO	O-C-N	-5.23	118.69	121.15

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	221	0
1	B	6295	0	6460	213	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	197	0	102	7	0
2	D	197	0	102	6	0
All	All	12999	0	13117	435	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 17.

All (435) 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:B:873:LEU:HD13	1:B:878:MET:HE2	1.72	0.72
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:271:GLY:O	1:B:277:LYS:NZ	2.19	0.69
1:B:440:ASN:ND2	1:B:451:GLU:OE2	2.25	0.69
1:B:318:MET:HE1	1:B:341:ILE:HD12	1.73	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:459:ILE:HA	1:B:463:LEU:HD12	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:800:MET:HE1	1:A:922:MET:HE1	1.80	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:796:ILE:HG22	1:A:800:MET:HE2	1.84	0.59
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
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: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:A:632:GLY:C	1:A:653:VAL:HG13	2.28	0.57
1:B:281:VAL:O	1:B:285:LEU:HD12	2.05	0.57
1:A:344:MET:HE1	1:A:352:GLU:OE2	2.04	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:B:632:GLY:C	1:B:653:VAL:HG23	2.33	0.54
1:A:838:GLY:H	1:A:842:SER:HG	1.53	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:A:626:LYS:NZ	1:A:670:PRO:O	2.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:675:ARG:HD3	1:B:677:TYR:CE2	2.44	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:792:TYR:OH	1:B:908:GLN:O	2.18	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
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:A:293:GLU:CD	1:A:294:ASP:H	2.18	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:B:800:MET:HE1	1:B:922:MET:HE1	1.93	0.51
1:B:842:SER:HB2	1:B:849:MET:HE2	1.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:258:MET:HE2	1:B:288:ALA:HB2	1.92	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
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:B:848:LEU:HD13	1:B:922:MET:HE2	1.95	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:848:LEU:HD13	1:A:922:MET:HE2	1.95	0.48
1:B:796:ILE:HG22	1:B:800:MET:HE2	1.94	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:286:TYR:CD2	1:B:318:MET:HE3	2.49	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:258:MET:HE1	1:A:285:LEU:HG	1.96	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:295:SER:O	1:B:295:SER:OG	2.32	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:1021:GLU:N	1:A:1021:GLU:CD	2.72	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:342:LYS:HE2	1:A:344:MET:HE3	1.95	0.47
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:A:907:MET:HE3	1:A:907:MET:HB2	1.68	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:764:LEU:HG	1:A:768:MET:HE3	1.96	0.46
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:754:MET:HE2	1:B:754:MET:HB3	1.66	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1021:GLU:CD	1:A:1021:GLU:H	2.25	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:844:LYS:C	1:A:919:ARG:HD3	2.43	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1136:MET:HE2	1:A:1136:MET:HB3	1.94	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:A:344:MET:HE3	1:A:344:MET:HB3	1.76	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:595:GLN:OE1	1:B:876:LYS:NZ	2.46	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:B:448:TYR:OH	1:B:477:GLU:OE2	2.33	0.42
1:B:844:LYS:C	1:B:919:ARG:HD3	2.45	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:948:TYR:OH	1:A:970:PRO:O	2.31	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
1:A:472:LEU:HD23	1:A:631:CYS:HG	1.85	0.41
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:838:GLY:C	1:B:839:GLN:HG2	2.45	0.41
1:B:351:LYS:HD3	1:B:351:LYS:HA	1.96	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: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
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

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	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

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%)	658 (95%)	32 (5%)	24	55
1	B	690/836 (82%)	653 (95%)	37 (5%)	20	49
All	All	1380/1672 (82%)	1311 (95%)	69 (5%)	22	51

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	LEU
1	A	331	TYR
1	A	344	MET
1	A	346	ASP
1	A	359	LEU
1	A	401	LEU
1	A	403	MET
1	A	414	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	677	TYR
1	A	696	ARG
1	A	699	GLU
1	A	725	GLU
1	A	783	LEU
1	A	803	ARG
1	A	804	GLU
1	A	844	LYS
1	A	859	GLU
1	A	869	GLN
1	A	874	ARG
1	A	904	ASP
1	A	913	SER
1	A	934	VAL
1	A	986	MET
1	A	1021	GLU
1	A	1053	ARG
1	A	1094	ARG
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	314	VAL
1	B	318	MET
1	B	326	SER
1	B	346	ASP
1	B	396	LEU
1	B	403	MET
1	B	408	ARG
1	B	410	GLU
1	B	415	ASN
1	B	427	LYS
1	B	430	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	449	SER
1	B	484	ARG
1	B	614	ASN
1	B	631	CYS
1	B	677	TYR
1	B	756	GLN
1	B	779	LYS
1	B	784	SER
1	B	843	LEU
1	B	863	CYS
1	B	874	ARG
1	B	941	ASP
1	B	982	THR
1	B	989	VAL
1	B	1011	LEU
1	B	1012	GLU
1	B	1043	VAL
1	B	1049	GLU
1	B	1051	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	438	HIS
1	A	440	ASN
1	A	660	GLN
1	A	787	HIS
1	B	236	ASN
1	B	280	GLN
1	B	660	GLN
1	B	1044	GLN

5.3.3 RNA ⓘ

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 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 [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%)	-0.62	0 100 100	30, 60, 101, 144	0
1	B	797/975 (81%)	-0.61	0 100 100	36, 63, 100, 132	0
2	C	10/10 (100%)	-0.98	0 100 100	49, 57, 93, 100	0
2	D	10/10 (100%)	-0.91	0 100 100	54, 66, 83, 87	0
All	All	1615/1970 (81%)	-0.62	0 100 100	30, 61, 100, 144	0

There are no RSRZ outliers to report.

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.