



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:18 pm BST

PDB ID : 3I7H  
Title : Crystal Structure of DDB1 in Complex with the H-Box Motif of HBX  
Authors : Li, T.; Robert, E.I.; Breugel, P.C.V.; Strubin, M.; Zheng, N.  
Deposited on : 2009-07-08  
Resolution : 2.90 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](mailto: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 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	:	2.11
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)	:	2.11

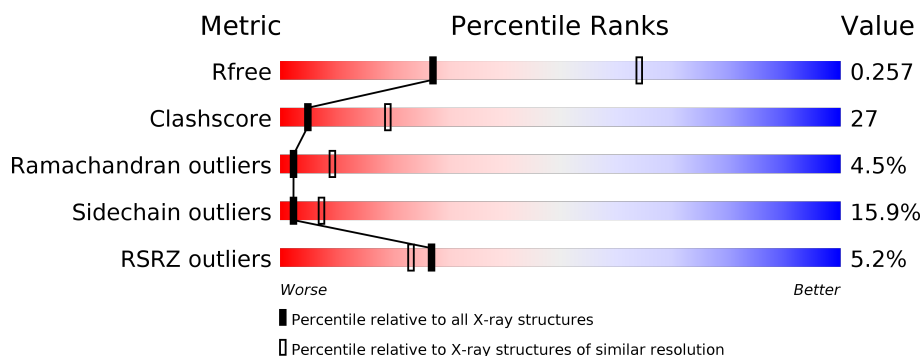
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1143	<div> <div>5%</div> <div> <div></div> <div>47%</div> <div>38%</div> <div>11%</div> <div>..</div> </div> </div>
2	B	14	<div> <div>7%</div> <div> <div></div> <div>50%</div> <div>29%</div> <div>21%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8837 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1114	Total	C	N	O	S	0	0	0
			8726	5529	1472	1677	48			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q16531
A	-1	SER	-	EXPRESSION TAG	UNP Q16531
A	0	HIS	-	EXPRESSION TAG	UNP Q16531
A	422	TYR	ASP	SEE REMARK 999	UNP Q16531
A	898	ASP	GLU	SEE REMARK 999	UNP Q16531
A	899	VAL	LEU	SEE REMARK 999	UNP Q16531

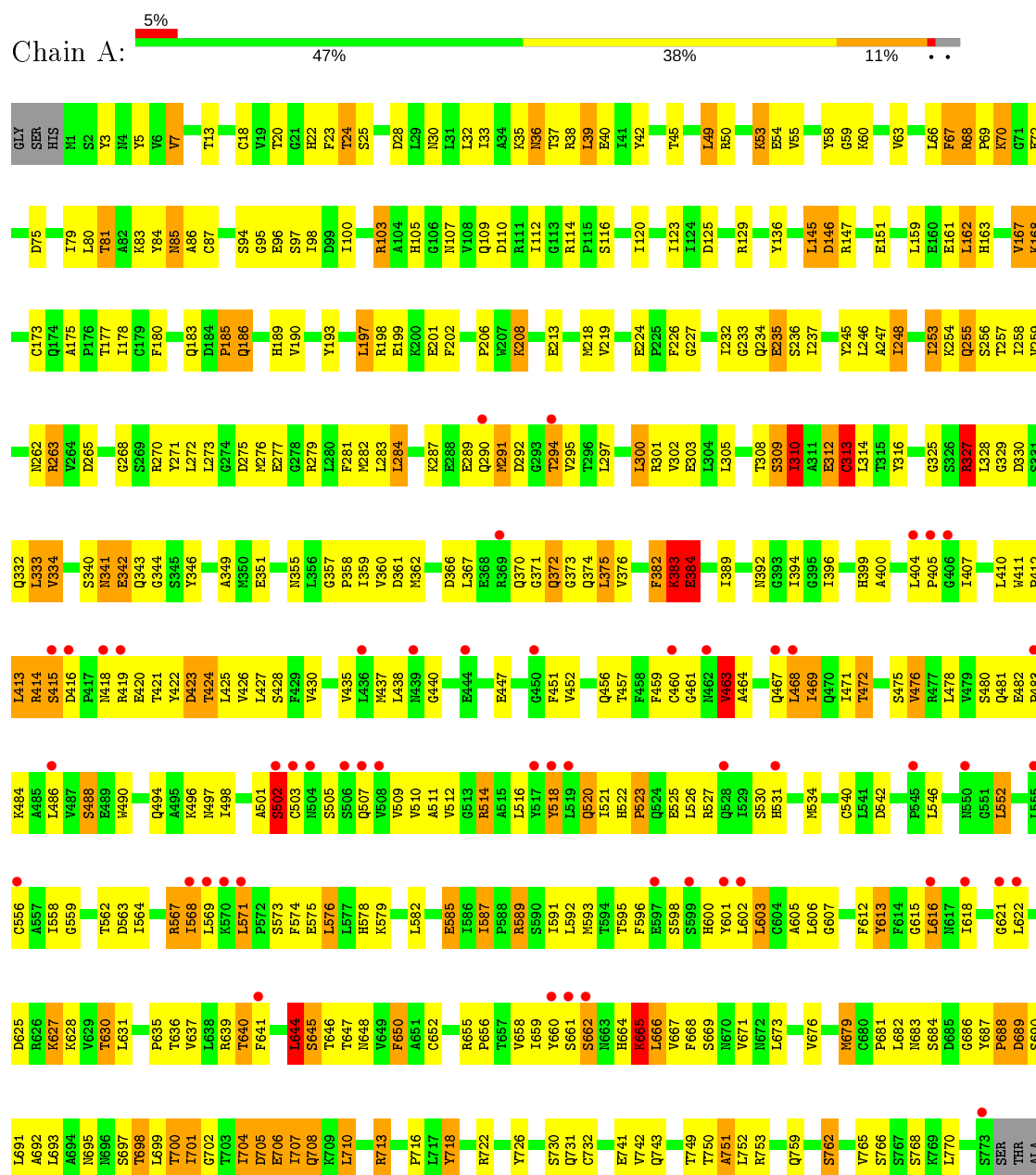
- Molecule 2 is a protein called X protein.

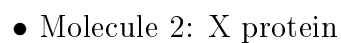
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	0	0	0
			111	73	21	17			

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: DNA damage-binding protein 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.86Å 132.86Å 183.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.90 48.78 – 2.68	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.80-2.90) 88.9 (48.78-2.68)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.234 , 0.279 0.232 , 0.257	Depositor DCC
$R_{free}$ test set	1909 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 67.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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	0.76	9/8885 (0.1%)	0.91	22/12034 (0.2%)
2	B	0.70	0/112	1.06	0/148
All	All	0.75	9/8997 (0.1%)	0.91	22/12182 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	LYS	CE-NZ	9.92	1.73	1.49
1	A	383	LYS	CB-CG	9.28	1.77	1.52
1	A	384	GLU	N-CA	8.67	1.63	1.46
1	A	313	CYS	CB-SG	-6.33	1.71	1.82
1	A	382	PHE	CD2-CE2	6.19	1.51	1.39
1	A	977	CYS	CB-SG	-5.74	1.72	1.81
1	A	718	TYR	CE1-CZ	5.63	1.45	1.38
1	A	718	TYR	CG-CD2	5.48	1.46	1.39
1	A	384	GLU	CG-CD	5.16	1.59	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	LYS	CB-CA-C	17.90	146.20	110.40
1	A	186	GLN	N-CA-CB	-14.99	83.62	110.60
1	A	841	ALA	N-CA-CB	-13.14	91.71	110.10
1	A	36	ASN	N-CA-C	-10.05	83.86	111.00
1	A	309	SER	N-CA-C	-9.38	85.68	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	840	GLU	N-CA-C	-7.46	90.85	111.00
1	A	856	GLY	N-CA-C	7.37	131.53	113.10
1	A	514	ARG	N-CA-CB	-6.87	98.24	110.60
1	A	514	ARG	N-CA-C	-6.57	93.26	111.00
1	A	185	PRO	N-CA-C	6.50	129.00	112.10
1	A	35	LYS	N-CA-C	-6.16	94.38	111.00
1	A	330	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	383	LYS	CG-CD-CE	-6.04	93.77	111.90
1	A	468	LEU	CA-CB-CG	5.88	128.84	115.30
1	A	308	THR	CB-CA-C	5.87	127.46	111.60
1	A	718	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	A	644	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	1000	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	327	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	710	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	841	ALA	N-CA-C	-5.27	96.78	111.00
1	A	552	LEU	CA-CB-CG	5.16	127.17	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	308	THR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	GLU	Peptide

## 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	8726	0	8706	478	0
2	B	111	0	131	9	0
All	All	8837	0	8837	485	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 27.

All (485) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:LYS:CG	1:A:383:LYS:CB	1.77	1.58
1:A:383:LYS:CE	1:A:383:LYS:NZ	1.73	1.50
1:A:907:ASN:HB2	1:A:942:PHE:CE2	1.69	1.27
1:A:928:ARG:HH21	1:A:953:TRP:HB2	1.11	1.13
1:A:660:TYR:HB2	1:A:667:VAL:HB	1.24	1.09
1:A:907:ASN:HB2	1:A:942:PHE:CZ	1.96	0.99
1:A:1032:THR:HG22	1:A:1034:ASN:H	1.30	0.97
1:A:270:ARG:HB3	1:A:282:MET:HE1	1.45	0.96
1:A:263:ARG:HB3	1:A:271:TYR:CE2	2.01	0.95
1:A:1061:VAL:HG21	1:A:1108:VAL:HG23	1.48	0.94
1:A:910:MET:O	1:A:910:MET:HG3	1.64	0.94
1:A:587:ILE:HD13	1:A:587:ILE:H	1.31	0.92
1:A:275:ASP:OD2	1:A:279:ARG:HD2	1.68	0.92
1:A:367:LEU:HB2	1:A:374:GLN:NE2	1.88	0.88
1:A:907:ASN:HA	1:A:942:PHE:HZ	1.41	0.86
1:A:1109:VAL:HG12	1:A:1109:VAL:O	1.75	0.85
1:A:255:GLN:OE1	1:A:279:ARG:NH2	2.08	0.85
1:A:894:THR:HG22	1:A:895:THR:H	1.39	0.85
1:A:23:PHE:H	1:A:30:ASN:ND2	1.75	0.84
1:A:907:ASN:CB	1:A:942:PHE:CE2	2.61	0.82
1:A:928:ARG:NH2	1:A:953:TRP:HB2	1.93	0.82
1:A:270:ARG:CB	1:A:282:MET:HE1	2.10	0.81
1:A:440:GLY:O	1:A:686:GLY:HA3	1.79	0.81
1:A:522:HIS:HB2	1:A:527:ARG:NH1	1.95	0.81
1:A:329:GLY:HA3	1:A:384:GLU:HG2	1.61	0.80
1:A:907:ASN:CB	1:A:942:PHE:CZ	2.64	0.80
1:A:457:THR:HG22	1:A:459:PHE:H	1.46	0.80
1:A:1108:VAL:O	1:A:1109:VAL:HB	1.81	0.80
1:A:3:TYR:HB3	1:A:1048:TYR:HB2	1.64	0.78
1:A:589:ARG:HG3	1:A:635:PRO:HB2	1.64	0.77
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.67	0.76
1:A:262:ASN:ND2	1:A:316:TYR:H	1.84	0.76
1:A:414:ARG:HA	1:A:422:TYR:HA	1.68	0.76
1:A:498:ILE:HA	1:A:512:VAL:HG22	1.68	0.76
1:A:129:ARG:NH2	1:A:197:LEU:HD21	2.02	0.75
1:A:841:ALA:HA	2:B:88:ILE:HG22	1.69	0.75
1:A:509:VAL:HG21	1:A:571:LEU:HD11	1.69	0.75
1:A:699:LEU:HD23	1:A:700:THR:N	2.02	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:GLU:HG3	1:A:707:ILE:N	2.02	0.74
1:A:95:GLY:C	1:A:97:SER:H	1.89	0.74
1:A:262:ASN:HD22	1:A:316:TYR:H	1.32	0.74
1:A:355:ASN:ND2	1:A:357:GLY:H	1.86	0.74
1:A:907:ASN:HA	1:A:942:PHE:CZ	2.22	0.74
1:A:290:GLN:O	1:A:292:ASP:N	2.21	0.73
1:A:870:VAL:HG11	1:A:873:MET:CE	2.18	0.73
1:A:660:TYR:HB2	1:A:667:VAL:CB	2.13	0.73
1:A:985:THR:HA	1:A:989:ARG:HB2	1.69	0.73
1:A:367:LEU:HB2	1:A:374:GLN:HE21	1.52	0.73
1:A:37:THR:HG22	1:A:59:GLY:O	1.88	0.73
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.72	0.71
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.23	0.71
1:A:1058:LEU:HD22	1:A:1062:ILE:CD1	2.21	0.70
1:A:38:ARG:HD2	1:A:54:GLU:OE1	1.90	0.70
1:A:909:ILE:HA	1:A:926:LEU:HD22	1.73	0.70
1:A:522:HIS:HB2	1:A:527:ARG:HH12	1.54	0.70
1:A:864:LYS:HB2	1:A:899:VAL:HG23	1.73	0.70
1:A:396:ILE:HD11	1:A:673:LEU:HD11	1.75	0.69
1:A:917:LYS:C	1:A:919:ASP:H	1.96	0.68
1:A:1058:LEU:HD22	1:A:1062:ILE:HD11	1.75	0.68
1:A:415:SER:HB2	1:A:423:ASP:OD2	1.93	0.68
1:A:879:LYS:HB3	1:A:891:TYR:O	1.94	0.68
1:A:894:THR:HG22	1:A:895:THR:N	2.08	0.68
1:A:1032:THR:HG22	1:A:1034:ASN:N	2.07	0.68
1:A:1061:VAL:CG2	1:A:1108:VAL:HG23	2.24	0.68
1:A:282:MET:HG2	1:A:305:LEU:HD11	1.73	0.67
1:A:270:ARG:HG2	1:A:284:LEU:HD23	1.77	0.67
1:A:660:TYR:CE2	1:A:707:ILE:HG12	2.29	0.67
1:A:392:ASN:HD22	1:A:1012:LEU:HB2	1.59	0.67
1:A:1050:LEU:O	1:A:1053:ASP:HB3	1.93	0.67
1:A:917:LYS:O	1:A:919:ASP:N	2.27	0.67
1:A:985:THR:O	1:A:986:ASP:HB2	1.95	0.67
1:A:81:THR:HG21	1:A:85:ASN:ND2	2.10	0.66
1:A:5:TYR:CE2	1:A:7:VAL:HG22	2.31	0.66
1:A:587:ILE:H	1:A:587:ILE:CD1	2.05	0.66
1:A:522:HIS:HB2	1:A:527:ARG:CZ	2.25	0.65
1:A:917:LYS:HG2	1:A:959:ILE:HG21	1.78	0.65
1:A:275:ASP:HB3	1:A:277:GLU:H	1.61	0.65
1:A:907:ASN:HD21	1:A:909:ILE:HB	1.60	0.65
1:A:1026:GLY:O	1:A:1041:THR:HG23	1.96	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:CG2	1:A:85:ASN:HD22	2.09	0.65
1:A:428:SER:OG	1:A:456:GLN:HG3	1.96	0.65
1:A:312:GLU:HG3	1:A:327:ARG:HD3	1.79	0.65
1:A:413:LEU:HB3	1:A:424:THR:HB	1.78	0.65
1:A:426:VAL:HG22	1:A:435:VAL:HG13	1.78	0.65
1:A:313:CYS:HB3	1:A:325:GLY:HA3	1.78	0.65
1:A:81:THR:HG21	1:A:85:ASN:HD22	1.60	0.65
1:A:562:THR:O	1:A:564:ILE:HD12	1.96	0.64
1:A:564:ILE:HG12	1:A:585:GLU:HA	1.78	0.64
1:A:662:SER:HB3	1:A:665:LYS:HB3	1.80	0.64
1:A:949:PHE:O	1:A:950:ASN:HB3	1.97	0.64
1:A:95:GLY:C	1:A:97:SER:N	2.51	0.64
1:A:272:LEU:O	1:A:273:LEU:HD23	1.98	0.64
1:A:854:SER:O	1:A:855:ASP:C	2.34	0.64
1:A:1111:ASN:HA	1:A:1124:ALA:HB1	1.80	0.64
1:A:564:ILE:HG22	1:A:564:ILE:O	1.98	0.64
1:A:659:ILE:HA	1:A:667:VAL:O	1.97	0.64
1:A:1125:THR:HB	1:A:1128:ASP:HB2	1.78	0.63
1:A:23:PHE:HB2	1:A:66:LEU:HD22	1.81	0.63
1:A:290:GLN:O	1:A:291:MET:C	2.36	0.63
1:A:888:VAL:HB	1:A:907:ASN:CG	2.19	0.63
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.81	0.63
1:A:907:ASN:CA	1:A:942:PHE:CZ	2.80	0.63
1:A:22:HIS:HD2	1:A:28:ASP:O	1.82	0.63
1:A:394:ILE:CG2	1:A:704:ILE:HD12	2.28	0.63
1:A:1123:GLU:O	1:A:1124:ALA:HB2	1.99	0.63
1:A:906:TYR:O	1:A:942:PHE:HE2	1.82	0.63
1:A:558:ILE:HG23	1:A:567:ARG:HG2	1.81	0.62
1:A:329:GLY:HA3	1:A:384:GLU:CG	2.30	0.62
1:A:452:VAL:HG21	1:A:472:THR:HG21	1.79	0.62
1:A:564:ILE:CD1	1:A:585:GLU:HA	2.29	0.62
1:A:864:LYS:HD2	1:A:899:VAL:O	2.00	0.62
1:A:70:LYS:H	1:A:70:LYS:CD	2.12	0.62
1:A:660:TYR:CZ	1:A:707:ILE:HA	2.34	0.62
1:A:1091:GLY:O	1:A:1095:GLU:HG3	2.00	0.62
1:A:928:ARG:HH11	1:A:928:ARG:HG3	1.64	0.61
1:A:213:GLU:OE1	1:A:233:GLY:HA3	1.99	0.61
1:A:490:TRP:HB2	1:A:526:LEU:HD13	1.81	0.61
1:A:921:ILE:HG22	1:A:922:LEU:H	1.65	0.61
1:A:616:LEU:HG	1:A:621:GLY:HA2	1.81	0.61
1:A:910:MET:H	1:A:926:LEU:HD13	1.65	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ILE:HG23	1:A:237:ILE:HG12	1.83	0.61
1:A:270:ARG:CG	1:A:282:MET:HE1	2.30	0.61
1:A:919:ASP:CG	1:A:920:PHE:H	2.04	0.61
1:A:985:THR:HG22	1:A:989:ARG:HD3	1.82	0.60
1:A:1032:THR:HG22	1:A:1033:VAL:N	2.16	0.60
1:A:906:TYR:O	1:A:942:PHE:CE2	2.54	0.60
1:A:1133:VAL:HA	1:A:1136:LEU:HD12	1.82	0.60
1:A:1048:TYR:O	1:A:1052:LEU:HB2	2.02	0.60
1:A:277:GLU:OE1	1:A:279:ARG:NH1	2.34	0.59
1:A:522:HIS:HB2	1:A:527:ARG:NH2	2.17	0.59
1:A:641:PHE:CZ	1:A:648:ASN:HB2	2.38	0.59
1:A:411:TRP:HB2	1:A:460:CYS:HB3	1.85	0.59
1:A:494:GLN:HB2	1:A:496:LYS:HE2	1.85	0.59
1:A:394:ILE:HG21	1:A:704:ILE:HD12	1.85	0.59
1:A:1088:PHE:O	1:A:1089:ILE:HG13	2.03	0.58
1:A:23:PHE:H	1:A:30:ASN:HD22	1.51	0.58
1:A:55:VAL:HG11	1:A:100:ILE:HG13	1.85	0.58
1:A:567:ARG:HB3	1:A:579:LYS:HB3	1.85	0.58
1:A:768:SER:OG	1:A:770:LEU:HB2	2.04	0.58
1:A:948:ASP:HB2	1:A:992:LEU:CD1	2.33	0.58
1:A:1051:LEU:HB3	1:A:1094:ILE:HD11	1.84	0.58
1:A:893:TRP:CE3	1:A:899:VAL:HG13	2.39	0.58
1:A:874:VAL:HG12	1:A:881:LEU:HD23	1.86	0.58
1:A:177:THR:HG21	1:A:206:PRO:HD2	1.86	0.58
1:A:375:LEU:HD23	1:A:376:VAL:N	2.19	0.58
1:A:573:SER:OG	1:A:575:GLU:HG2	2.04	0.58
1:A:13:THR:OG1	1:A:355:ASN:ND2	2.35	0.58
1:A:49:LEU:HD13	1:A:333:LEU:HD21	1.84	0.58
1:A:1045:GLU:HG2	1:A:1046:SER:N	2.19	0.58
1:A:606:LEU:HD11	1:A:612:PHE:HE1	1.68	0.57
1:A:70:LYS:HD3	1:A:70:LYS:H	1.69	0.57
1:A:948:ASP:HB2	1:A:992:LEU:HD12	1.85	0.57
1:A:798:THR:OG1	1:A:800:GLU:HG2	2.03	0.57
1:A:197:LEU:H	1:A:197:LEU:CD2	2.18	0.57
1:A:83:LYS:O	1:A:84:TYR:HB2	2.04	0.57
1:A:1013:VAL:HG11	1:A:1138:ARG:O	2.04	0.57
1:A:568:ILE:O	1:A:569:LEU:HD23	2.04	0.57
1:A:641:PHE:CE2	1:A:650:PHE:HB2	2.40	0.57
1:A:917:LYS:HD2	1:A:921:ILE:HD12	1.86	0.57
1:A:969:GLU:HG2	1:A:970:ASN:N	2.19	0.57
1:A:1011:SER:OG	1:A:1013:VAL:HG23	2.04	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:SER:H	1:A:664:HIS:HE1	1.53	0.56
1:A:1108:VAL:HG12	1:A:1109:VAL:HG23	1.86	0.56
1:A:518:TYR:HB2	1:A:574:PHE:CZ	2.41	0.56
1:A:716:PRO:HB2	1:A:718:TYR:CE1	2.41	0.56
1:A:5:TYR:HE2	1:A:7:VAL:HG22	1.70	0.56
1:A:396:ILE:HG23	1:A:704:ILE:HD13	1.86	0.56
1:A:24:THR:CG2	1:A:28:ASP:OD1	2.53	0.56
1:A:405:PRO:HA	1:A:697:SER:HA	1.87	0.56
1:A:984:THR:HG22	1:A:987:GLU:HB3	1.87	0.56
1:A:23:PHE:HB2	1:A:66:LEU:CD2	2.36	0.56
1:A:690:SER:OG	1:A:691:LEU:N	2.34	0.56
1:A:641:PHE:HE2	1:A:650:PHE:HB2	1.71	0.55
1:A:1110:ALA:O	1:A:1111:ASN:HB3	2.06	0.55
1:A:359:ILE:HG13	1:A:1035:GLY:HA2	1.87	0.55
1:A:659:ILE:HG12	1:A:668:PHE:CE1	2.41	0.55
1:A:641:PHE:HA	1:A:681:PRO:HG3	1.88	0.55
1:A:546:LEU:HB3	1:A:618:ILE:HG21	1.89	0.55
1:A:639:ARG:HG3	1:A:640:THR:N	2.21	0.55
1:A:925:ASP:OD1	1:A:925:ASP:C	2.44	0.55
1:A:332:GLN:HB2	1:A:351:GLU:O	2.06	0.55
1:A:81:THR:HG22	1:A:85:ASN:H	1.72	0.55
1:A:762:SER:O	1:A:803:HIS:HA	2.07	0.55
1:A:383:LYS:CB	1:A:383:LYS:CD	2.79	0.55
1:A:24:THR:HG21	1:A:28:ASP:OD1	2.06	0.54
1:A:341:ASN:OD1	1:A:342:GLU:O	2.26	0.54
1:A:568:ILE:HG12	1:A:578:HIS:O	2.07	0.54
1:A:731:GLN:O	1:A:796:GLN:HG2	2.07	0.54
1:A:1032:THR:HB	1:A:1036:MET:H	1.71	0.54
1:A:414:ARG:CA	1:A:422:TYR:HA	2.37	0.54
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.72	0.54
1:A:592:LEU:C	1:A:602:LEU:HD12	2.28	0.54
1:A:591:ILE:HG13	1:A:603:LEU:O	2.08	0.54
1:A:542:ASP:OD1	1:A:593:MET:HG2	2.08	0.54
1:A:984:THR:O	1:A:986:ASP:N	2.41	0.54
1:A:469:ILE:HD11	1:A:471:ILE:CG1	2.38	0.54
1:A:558:ILE:HG23	1:A:567:ARG:CG	2.38	0.54
1:A:692:ALA:C	1:A:693:LEU:HD12	2.29	0.53
1:A:750:THR:O	1:A:751:ALA:HB2	2.09	0.53
1:A:917:LYS:C	1:A:919:ASP:N	2.60	0.53
1:A:24:THR:H	1:A:30:ASN:HD21	1.56	0.53
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ILE:N	1:A:389:ILE:HD12	2.24	0.53
1:A:518:TYR:HB3	1:A:530:SER:HB2	1.90	0.53
1:A:917:LYS:HB2	1:A:921:ILE:HG13	1.89	0.53
1:A:1023:PRO:O	1:A:1024:THR:HG23	2.09	0.53
1:A:95:GLY:O	1:A:97:SER:N	2.42	0.53
1:A:340:SER:HB3	1:A:346:TYR:CZ	2.44	0.53
1:A:690:SER:O	1:A:691:LEU:HG	2.09	0.53
1:A:72:GLU:OE2	1:A:103:ARG:NH2	2.41	0.53
1:A:291:MET:O	1:A:292:ASP:HB2	2.09	0.52
1:A:373:GLY:HA3	1:A:1011:SER:O	2.09	0.52
1:A:478:LEU:HD21	1:A:521:ILE:HG23	1.89	0.52
1:A:279:ARG:HD3	1:A:281:PHE:CZ	2.44	0.52
1:A:596:PHE:HE2	1:A:647:THR:O	1.92	0.52
1:A:396:ILE:HD11	1:A:673:LEU:HD21	1.91	0.52
1:A:263:ARG:HB3	1:A:271:TYR:CD2	2.45	0.52
1:A:105:HIS:O	1:A:151:GLU:HA	2.10	0.52
1:A:695:ASN:OD1	1:A:698:THR:N	2.37	0.52
1:A:1109:VAL:O	1:A:1109:VAL:CG1	2.46	0.52
1:A:639:ARG:HG2	1:A:679:MET:SD	2.50	0.52
1:A:949:PHE:H	1:A:949:PHE:HD1	1.58	0.52
1:A:291:MET:HG3	1:A:291:MET:O	2.10	0.51
1:A:177:THR:HG21	1:A:206:PRO:CD	2.41	0.51
1:A:270:ARG:HB3	1:A:282:MET:CE	2.29	0.51
1:A:598:SER:H	1:A:664:HIS:CE1	2.28	0.51
1:A:564:ILE:CG1	1:A:585:GLU:HA	2.39	0.51
1:A:197:LEU:H	1:A:197:LEU:HD23	1.75	0.51
1:A:18:CYS:HA	1:A:32:LEU:O	2.11	0.51
1:A:838:PRO:O	1:A:839:GLU:HG3	2.11	0.51
1:A:253:ILE:CD1	1:A:258:ILE:HD11	2.41	0.51
1:A:265:ASP:OD2	1:A:270:ARG:NE	2.36	0.51
1:A:253:ILE:HG12	1:A:258:ILE:HD11	1.93	0.51
1:A:644:LEU:HD11	1:A:707:ILE:HD11	1.93	0.51
1:A:270:ARG:HA	1:A:283:LEU:O	2.12	0.50
1:A:613:TYR:O	1:A:625:ASP:O	2.29	0.50
1:A:312:GLU:CG	1:A:327:ARG:HD3	2.42	0.50
1:A:848:ILE:O	1:A:863:GLU:O	2.28	0.50
1:A:1055:GLN:HE21	1:A:1089:ILE:HG23	1.76	0.50
1:A:636:THR:HA	1:A:652:CYS:O	2.11	0.50
1:A:7:VAL:HG11	1:A:1140:HIS:HE1	1.76	0.50
1:A:605:ALA:HB1	1:A:636:THR:HB	1.93	0.50
1:A:936:LYS:HG3	1:A:943:GLU:HB2	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:LEU:HD22	1:A:1094:ILE:HD13	1.94	0.50
1:A:907:ASN:ND2	1:A:909:ILE:HB	2.26	0.50
1:A:852:GLN:N	1:A:859:GLN:O	2.39	0.50
1:A:661:SER:HA	1:A:665:LYS:O	2.12	0.50
1:A:1002:GLU:HB3	1:A:1032:THR:HG23	1.94	0.50
1:A:820:LYS:HG2	1:A:826:ASN:O	2.12	0.50
1:A:1123:GLU:O	1:A:1124:ALA:CB	2.59	0.49
1:A:123:ILE:HD11	1:A:178:ILE:HD11	1.94	0.49
1:A:22:HIS:CD2	1:A:28:ASP:O	2.63	0.49
1:A:732:CYS:HB2	1:A:794:ILE:O	2.12	0.49
1:A:870:VAL:HG11	1:A:873:MET:HE2	1.92	0.49
1:A:360:VAL:HG22	2:B:97:THR:HG23	1.94	0.49
1:A:309:SER:O	1:A:310:ILE:C	2.51	0.49
1:A:501:ALA:O	1:A:502:SER:HB2	2.12	0.49
1:A:1010:GLY:O	1:A:1027:SER:OG	2.31	0.49
1:A:173:CYS:HB3	1:A:175:ALA:O	2.13	0.49
1:A:910:MET:HB3	1:A:926:LEU:HD13	1.94	0.49
1:A:949:PHE:N	1:A:949:PHE:CD1	2.80	0.49
1:A:1062:ILE:HG22	1:A:1063:LYS:O	2.12	0.49
1:A:263:ARG:CB	1:A:271:TYR:CE2	2.86	0.49
1:A:276:MET:O	1:A:310:ILE:CD1	2.60	0.49
1:A:301:ARG:NH1	1:A:303:GLU:OE2	2.45	0.49
1:A:630:THR:O	1:A:631:LEU:HD23	2.12	0.49
1:A:1097:PHE:HE2	1:A:1130:ILE:HA	1.77	0.49
1:A:546:LEU:HD13	1:A:618:ILE:HG22	1.95	0.49
1:A:342:GLU:C	1:A:344:GLY:H	2.16	0.49
1:A:852:GLN:O	1:A:859:GLN:N	2.39	0.49
1:A:511:ALA:HB2	1:A:516:LEU:HD23	1.95	0.49
1:A:1048:TYR:CE2	1:A:1052:LEU:HD12	2.48	0.48
1:A:836:VAL:HG12	1:A:836:VAL:O	2.13	0.48
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.94	0.48
1:A:923:VAL:CG2	1:A:959:ILE:HG13	2.43	0.48
1:A:245:TYR:CE2	1:A:247:ALA:HB2	2.48	0.48
1:A:334:VAL:HG22	1:A:349:ALA:HA	1.94	0.48
1:A:741:GLU:HG2	1:A:751:ALA:HA	1.94	0.48
1:A:931:LEU:HD23	1:A:947:ARG:HG3	1.94	0.48
1:A:1013:VAL:O	1:A:1014:MET:O	2.31	0.48
1:A:484:LYS:O	1:A:484:LYS:HG3	2.14	0.48
1:A:602:LEU:HG	1:A:603:LEU:N	2.27	0.48
1:A:828:TYR:CE2	1:A:852:GLN:HG3	2.48	0.48
1:A:80:LEU:HD23	1:A:120:ILE:HG21	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:HA	1:A:425:LEU:HD12	1.96	0.48
1:A:469:ILE:HD11	1:A:471:ILE:HG13	1.95	0.48
1:A:569:LEU:HD22	1:A:576:LEU:HA	1.95	0.48
1:A:1032:THR:OG1	1:A:1036:MET:HB3	2.14	0.48
1:A:1098:LEU:HD21	1:A:1133:VAL:HB	1.94	0.48
1:A:435:VAL:HB	1:A:447:GLU:HA	1.96	0.48
1:A:612:PHE:CE2	1:A:628:LYS:HB2	2.49	0.48
1:A:704:ILE:HA	1:A:704:ILE:HD13	1.75	0.48
1:A:107:ASN:OD1	1:A:109:GLN:HB2	2.13	0.48
1:A:333:LEU:HB2	1:A:351:GLU:HB3	1.96	0.48
1:A:743:GLN:HB3	1:A:783:GLY:N	2.28	0.48
1:A:199:GLU:HG3	1:A:201:GLU:HG3	1.95	0.47
1:A:23:PHE:H	1:A:30:ASN:HD21	1.58	0.47
1:A:24:THR:HB	1:A:30:ASN:OD1	2.14	0.47
1:A:480:SER:OG	1:A:483:PRO:HB2	2.14	0.47
1:A:40:GLU:HB3	1:A:42:TYR:HE1	1.80	0.47
1:A:45:THR:HG21	1:A:50:ARG:HD2	1.97	0.47
1:A:399:HIS:CE1	1:A:702:GLY:HA2	2.49	0.47
1:A:463:VAL:HA	1:A:505:SER:O	2.14	0.47
1:A:389:ILE:HD13	1:A:713:ARG:HB3	1.97	0.47
1:A:459:PHE:CE1	1:A:503:CYS:HB3	2.49	0.47
1:A:540:CYS:SG	1:A:559:GLY:HA3	2.54	0.47
1:A:658:VAL:HG23	1:A:671:VAL:CG2	2.45	0.47
1:A:706:GLU:HG3	1:A:707:ILE:H	1.76	0.47
1:A:262:ASN:HB2	1:A:314:LEU:O	2.14	0.47
1:A:362:MET:HG2	1:A:1006:VAL:HG11	1.95	0.47
1:A:414:ARG:HB2	1:A:422:TYR:HA	1.97	0.47
1:A:516:LEU:O	1:A:531:HIS:HA	2.14	0.47
1:A:613:TYR:HE2	1:A:627:LYS:O	1.97	0.47
1:A:722:ARG:NH1	1:A:789:HIS:HE1	2.12	0.47
2:B:88:ILE:HD12	2:B:90:PRO:HD2	1.96	0.47
1:A:507:GLN:OE1	1:A:552:LEU:HA	2.15	0.47
1:A:1058:LEU:HD22	1:A:1062:ILE:HD12	1.94	0.47
1:A:414:ARG:HD3	1:A:419:ARG:O	2.14	0.47
1:A:684:SER:O	1:A:688:PRO:HG3	2.15	0.47
1:A:226:PHE:CZ	1:A:287:LYS:HG2	2.50	0.46
1:A:85:ASN:H	1:A:85:ASN:HD22	1.62	0.46
1:A:691:LEU:O	1:A:701:ILE:HA	2.16	0.46
1:A:177:THR:HG21	1:A:206:PRO:HG2	1.96	0.46
1:A:1076:PHE:CE2	1:A:1078:THR:HG23	2.50	0.46
1:A:234:GLN:O	1:A:236:SER:N	2.48	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:PHE:CD2	1:A:650:PHE:C	2.88	0.46
1:A:294:THR:HG22	1:A:295:VAL:H	1.81	0.46
1:A:741:GLU:HB3	1:A:749:THR:HB	1.96	0.46
1:A:954:MET:HE2	1:A:957:VAL:HG23	1.98	0.46
1:A:18:CYS:N	1:A:313:CYS:SG	2.88	0.46
1:A:947:ARG:HG2	1:A:948:ASP:N	2.30	0.46
1:A:163:HIS:CD2	1:A:183:GLN:HB3	2.51	0.46
1:A:644:LEU:H	1:A:644:LEU:HD23	1.79	0.46
1:A:22:HIS:O	1:A:75:ASP:HB2	2.16	0.46
1:A:923:VAL:HG21	1:A:959:ILE:HG13	1.97	0.46
1:A:382:PHE:C	1:A:384:GLU:H	2.18	0.46
2:B:88:ILE:O	2:B:88:ILE:HG13	2.14	0.46
1:A:1061:VAL:HG11	1:A:1104:LYS:HB3	1.98	0.46
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.98	0.45
1:A:839:GLU:N	1:A:840:GLU:OE1	2.48	0.45
1:A:482:GLU:HB3	1:A:483:PRO:HD3	1.99	0.45
1:A:641:PHE:HZ	1:A:648:ASN:HB2	1.80	0.45
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.51	0.45
1:A:161:GLU:OE1	1:A:193:TYR:OH	2.28	0.45
1:A:63:VAL:HB	1:A:80:LEU:HB3	1.99	0.45
1:A:464:ALA:O	1:A:467:GLN:HB2	2.16	0.45
1:A:598:SER:HB2	1:A:664:HIS:NE2	2.31	0.45
1:A:688:PRO:O	1:A:689:ASP:C	2.54	0.45
1:A:370:GLN:O	1:A:372:GLN:N	2.48	0.45
1:A:885:ASN:O	1:A:886:SER:HB2	2.16	0.45
1:A:83:LYS:HE2	1:A:1073:TRP:O	2.17	0.45
1:A:512:VAL:O	1:A:512:VAL:HG12	2.17	0.45
1:A:708:GLN:HB2	1:A:710:LEU:O	2.16	0.45
2:B:99:GLY:O	2:B:101:SER:N	2.50	0.45
1:A:110:ASP:HB2	1:A:136:TYR:CE1	2.52	0.45
1:A:69:PRO:HG2	1:A:72:GLU:HG3	1.98	0.45
1:A:63:VAL:O	1:A:79:ILE:HA	2.17	0.45
1:A:3:TYR:HB3	1:A:1048:TYR:CB	2.41	0.45
1:A:459:PHE:HE2	1:A:461:GLY:HA3	1.82	0.45
1:A:208:LYS:CE	1:A:208:LYS:H	2.29	0.45
1:A:475:SER:HB2	1:A:490:TRP:O	2.17	0.45
1:A:893:TRP:HE3	1:A:899:VAL:HG13	1.82	0.45
1:A:985:THR:HA	1:A:989:ARG:CB	2.44	0.44
1:A:33:ILE:HB	1:A:40:GLU:HB2	2.00	0.44
1:A:520:GLN:HB3	1:A:527:ARG:HH11	1.80	0.44
1:A:263:ARG:CG	1:A:263:ARG:HH11	2.30	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:GLU:OE1	1:A:789:HIS:NE2	2.47	0.44
1:A:480:SER:O	1:A:484:LYS:HA	2.16	0.44
1:A:907:ASN:HD21	1:A:909:ILE:CB	2.29	0.44
1:A:1024:THR:OG1	1:A:1139:ILE:HD11	2.18	0.44
1:A:270:ARG:HG2	1:A:282:MET:HE1	1.99	0.44
1:A:645:SER:OG	1:A:646:THR:N	2.49	0.44
1:A:750:THR:O	1:A:751:ALA:CB	2.66	0.44
1:A:742:VAL:HG12	1:A:785:GLU:HG2	2.00	0.44
1:A:732:CYS:SG	1:A:793:ILE:HG23	2.57	0.44
1:A:916:THR:OG1	1:A:922:LEU:HD12	2.18	0.44
1:A:1032:THR:CG2	1:A:1033:VAL:N	2.79	0.44
1:A:234:GLN:C	1:A:235:GLU:HG2	2.38	0.44
1:A:36:ASN:HB3	1:A:37:THR:H	1.66	0.44
1:A:399:HIS:HB3	1:A:687:TYR:HE1	1.83	0.44
1:A:69:PRO:O	1:A:72:GLU:HB2	2.18	0.44
1:A:68:ARG:NE	1:A:75:ASP:OD2	2.50	0.44
1:A:1045:GLU:CG	1:A:1046:SER:N	2.80	0.44
1:A:328:LEU:HA	1:A:358:PRO:HD3	1.99	0.44
1:A:478:LEU:O	1:A:486:LEU:HA	2.18	0.44
1:A:1110:ALA:O	1:A:1111:ASN:CB	2.66	0.44
1:A:129:ARG:O	1:A:145:LEU:HB2	2.18	0.44
1:A:1102:ARG:HH21	1:A:1106:GLN:HE21	1.66	0.43
1:A:394:ILE:HG12	1:A:669:SER:OG	2.18	0.43
1:A:1002:GLU:OE1	1:A:1032:THR:HG21	2.18	0.43
1:A:39:LEU:HD12	1:A:40:GLU:N	2.33	0.43
1:A:690:SER:C	1:A:691:LEU:HG	2.38	0.43
1:A:370:GLN:C	1:A:372:GLN:H	2.22	0.43
1:A:437:MET:SD	1:A:438:LEU:N	2.92	0.43
1:A:731:GLN:HA	1:A:796:GLN:NE2	2.32	0.43
1:A:7:VAL:HG11	1:A:1140:HIS:CE1	2.52	0.43
1:A:355:ASN:CG	1:A:357:GLY:H	2.22	0.43
1:A:372:GLN:OE1	1:A:372:GLN:C	2.56	0.43
1:A:932:LEU:HA	1:A:932:LEU:HD12	1.76	0.43
2:B:99:GLY:C	2:B:101:SER:H	2.21	0.43
1:A:1053:ASP:O	1:A:1054:MET:C	2.57	0.43
1:A:180:PHE:O	1:A:190:VAL:HA	2.18	0.43
1:A:592:LEU:O	1:A:602:LEU:HA	2.19	0.43
1:A:986:ASP:O	1:A:987:GLU:HB2	2.19	0.43
1:A:600:HIS:CG	1:A:618:ILE:HG23	2.52	0.43
2:B:94:HIS:O	2:B:97:THR:HG22	2.18	0.43
1:A:1024:THR:HB	1:A:1041:THR:HG21	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:SER:HB2	1:A:483:PRO:HD2	2.00	0.43
1:A:518:TYR:HB2	1:A:574:PHE:HZ	1.82	0.43
1:A:60:LYS:HE3	1:A:1001:GLY:O	2.18	0.43
1:A:892:GLU:O	1:A:899:VAL:HA	2.18	0.43
1:A:460:CYS:O	1:A:460:CYS:SG	2.76	0.43
1:A:563:ASP:OD2	1:A:567:ARG:NH1	2.52	0.43
1:A:1090:ASP:O	1:A:1093:LEU:N	2.52	0.43
1:A:984:THR:CG2	1:A:987:GLU:HB3	2.49	0.43
1:A:362:MET:HB2	1:A:375:LEU:HD21	1.99	0.42
1:A:361:ASP:OD1	1:A:362:MET:N	2.52	0.42
1:A:851:PHE:HB3	1:A:858:LEU:HD21	2.01	0.42
1:A:964:ASN:OD1	1:A:978:GLN:HG3	2.18	0.42
1:A:407:ILE:HG21	1:A:427:LEU:HD22	2.01	0.42
1:A:469:ILE:HD11	1:A:471:ILE:HG12	2.00	0.42
1:A:595:THR:HG23	1:A:600:HIS:HE1	1.83	0.42
1:A:616:LEU:HD12	1:A:622:LEU:O	2.19	0.42
1:A:631:LEU:C	1:A:655:ARG:HE	2.20	0.42
1:A:168:LYS:CD	1:A:219:VAL:O	2.67	0.42
1:A:39:LEU:C	1:A:39:LEU:HD12	2.38	0.42
1:A:58:TYR:CE2	1:A:1070:HIS:HB2	2.54	0.42
1:A:906:TYR:HD1	1:A:907:ASN:N	2.18	0.42
1:A:400:ALA:HB3	1:A:701:ILE:HD11	2.00	0.42
1:A:1055:GLN:HE22	1:A:1089:ILE:HA	1.83	0.42
1:A:226:PHE:HB3	1:A:297:LEU:CD1	2.49	0.42
1:A:310:ILE:HG12	1:A:310:ILE:H	1.28	0.42
1:A:830:ILE:HG12	1:A:850:VAL:HG22	2.02	0.42
1:A:234:GLN:NE2	1:A:257:THR:OG1	2.52	0.42
1:A:302:VAL:O	1:A:303:GLU:HG3	2.19	0.42
1:A:5:TYR:O	1:A:1040:VAL:HA	2.19	0.42
1:A:412:PRO:O	1:A:413:LEU:HB2	2.19	0.42
1:A:942:PHE:O	1:A:942:PHE:CD1	2.72	0.42
2:B:99:GLY:C	2:B:101:SER:N	2.73	0.42
1:A:562:THR:O	1:A:564:ILE:CD1	2.66	0.42
1:A:661:SER:HA	1:A:666:LEU:HA	2.01	0.42
1:A:933:LEU:HA	1:A:943:GLU:O	2.19	0.42
1:A:518:TYR:CE1	1:A:571:LEU:HD23	2.55	0.42
1:A:262:ASN:ND2	1:A:316:TYR:N	2.61	0.41
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.55	0.41
1:A:641:PHE:HA	1:A:681:PRO:CG	2.50	0.41
1:A:1051:LEU:HB3	1:A:1094:ILE:CD1	2.48	0.41
1:A:478:LEU:HD13	1:A:488:SER:HB3	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:HIS:HB2	1:A:527:ARG:HH22	1.81	0.41
1:A:907:ASN:HD21	1:A:909:ILE:CG1	2.33	0.41
1:A:958:GLU:OE2	1:A:1009:HIS:CD2	2.74	0.41
1:A:376:VAL:HG23	1:A:376:VAL:O	2.20	0.41
1:A:522:HIS:H	1:A:527:ARG:HH12	1.67	0.41
1:A:596:PHE:CE2	1:A:647:THR:O	2.71	0.41
1:A:24:THR:HG22	1:A:25:SER:N	2.36	0.41
1:A:514:ARG:O	1:A:534:MET:N	2.38	0.41
1:A:595:THR:HG23	1:A:600:HIS:CE1	2.55	0.41
1:A:809:GLN:HB3	1:A:810:ASN:ND2	2.35	0.41
1:A:358:PRO:HA	1:A:1033:VAL:O	2.20	0.41
1:A:589:ARG:HD2	1:A:637:VAL:HG22	2.03	0.41
1:A:129:ARG:HH22	1:A:197:LEU:HD21	1.81	0.41
1:A:53:LYS:HE2	1:A:53:LYS:HA	2.02	0.41
1:A:67:PHE:CD2	1:A:67:PHE:N	2.89	0.41
2:B:88:ILE:HD11	2:B:91:LYS:HG3	2.03	0.41
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	2.03	0.41
1:A:601:TYR:HA	1:A:615:GLY:HA2	2.02	0.41
1:A:766:SER:HB3	1:A:808:LEU:HD23	2.02	0.41
1:A:705:ASP:O	1:A:706:GLU:O	2.37	0.41
1:A:362:MET:HG2	1:A:1006:VAL:CG1	2.51	0.41
1:A:522:HIS:O	1:A:523:PRO:C	2.59	0.41
1:A:857:LYS:HE3	1:A:857:LYS:HB2	1.80	0.41
1:A:1055:GLN:NE2	1:A:1089:ILE:HG23	2.36	0.41
1:A:24:THR:CG2	1:A:25:SER:N	2.82	0.40
1:A:248:ILE:HG12	1:A:300:LEU:HD12	2.03	0.40
1:A:309:SER:HA	1:A:384:GLU:OE2	2.21	0.40
1:A:681:PRO:HA	1:A:691:LEU:HD23	2.03	0.40
1:A:830:ILE:HD13	1:A:880:LEU:HD13	2.02	0.40
1:A:919:ASP:CG	1:A:920:PHE:N	2.71	0.40
1:A:892:GLU:HB3	1:A:900:ARG:HG3	2.02	0.40
1:A:86:ALA:O	1:A:87:CYS:HB3	2.21	0.40
1:A:265:ASP:O	1:A:268:GLY:N	2.51	0.40
1:A:226:PHE:CE2	1:A:287:LYS:HG2	2.57	0.40
1:A:888:VAL:HB	1:A:907:ASN:CB	2.52	0.40
1:A:83:LYS:HB3	1:A:1072:PHE:HE2	1.87	0.40
1:A:518:TYR:CD2	1:A:518:TYR:C	2.95	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	1106/1143 (97%)	893 (81%)	164 (15%)	49 (4%)	2	10
2	B	12/14 (86%)	9 (75%)	2 (17%)	1 (8%)	1	2
All	All	1118/1157 (97%)	902 (81%)	166 (15%)	50 (4%)	2	9

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASP
1	A	235	GLU
1	A	256	SER
1	A	291	MET
1	A	523	PRO
1	A	683	ASN
1	A	706	GLU
1	A	751	ALA
1	A	864	LYS
1	A	985	THR
1	A	986	ASP
1	A	1014	MET
1	A	1123	GLU
1	A	1124	ALA
1	A	96	GLU
1	A	162	LEU
1	A	227	GLY
1	A	341	ASN
1	A	342	GLU
1	A	430	VAL
1	A	502	SER
1	A	644	LEU
1	A	689	ASP
1	A	707	ILE
1	A	855	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	918	GLY
1	A	987	GLU
1	A	1065	VAL
1	A	255	GLN
1	A	371	GLY
1	A	662	SER
1	A	413	LEU
1	A	463	VAL
1	A	950	ASN
1	A	970	ASN
1	A	1013	VAL
1	A	1053	ASP
1	A	1091	GLY
1	A	94	SER
1	A	420	GLU
1	A	665	LYS
1	A	688	PRO
1	A	838	PRO
1	A	185	PRO
1	A	951	PRO
1	A	1054	MET
1	A	1130	ILE
1	A	1109	VAL
1	A	310	ILE
2	B	99	GLY

### 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	977/1001 (98%)	822 (84%)	155 (16%)	2	7
2	B	13/13 (100%)	11 (85%)	2 (15%)	2	8
All	All	990/1014 (98%)	833 (84%)	157 (16%)	2	7

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	20	THR
1	A	24	THR
1	A	39	LEU
1	A	49	LEU
1	A	53	LYS
1	A	67	PHE
1	A	68	ARG
1	A	70	LYS
1	A	81	THR
1	A	85	ASN
1	A	98	ILE
1	A	103	ARG
1	A	112	ILE
1	A	114	ARG
1	A	116	SER
1	A	125	ASP
1	A	145	LEU
1	A	146	ASP
1	A	147	ARG
1	A	159	LEU
1	A	162	LEU
1	A	167	VAL
1	A	168	LYS
1	A	186	GLN
1	A	189	HIS
1	A	197	LEU
1	A	198	ARG
1	A	202	PHE
1	A	208	LYS
1	A	218	MET
1	A	224	GLU
1	A	246	LEU
1	A	248	ILE
1	A	253	ILE
1	A	254	LYS
1	A	259	VAL
1	A	263	ARG
1	A	284	LEU
1	A	289	GLU
1	A	294	THR
1	A	300	LEU
1	A	310	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	313	CYS
1	A	327	ARG
1	A	333	LEU
1	A	334	VAL
1	A	343	GLN
1	A	366	ASP
1	A	372	GLN
1	A	375	LEU
1	A	383	LYS
1	A	384	GLU
1	A	404	LEU
1	A	410	LEU
1	A	414	ARG
1	A	415	SER
1	A	416	ASP
1	A	418	ASN
1	A	421	THR
1	A	423	ASP
1	A	424	THR
1	A	451	PHE
1	A	463	VAL
1	A	468	LEU
1	A	469	ILE
1	A	472	THR
1	A	476	VAL
1	A	481	GLN
1	A	488	SER
1	A	497	ASN
1	A	502	SER
1	A	510	VAL
1	A	518	TYR
1	A	520	GLN
1	A	525	GLU
1	A	556	CYS
1	A	567	ARG
1	A	568	ILE
1	A	571	LEU
1	A	576	LEU
1	A	582	LEU
1	A	585	GLU
1	A	587	ILE
1	A	589	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	603	LEU
1	A	613	TYR
1	A	616	LEU
1	A	627	LYS
1	A	630	THR
1	A	640	THR
1	A	644	LEU
1	A	645	SER
1	A	650	PHE
1	A	665	LYS
1	A	666	LEU
1	A	676	VAL
1	A	679	MET
1	A	682	LEU
1	A	698	THR
1	A	700	THR
1	A	701	ILE
1	A	704	ILE
1	A	705	ASP
1	A	708	GLN
1	A	713	ARG
1	A	730	SER
1	A	752	LEU
1	A	753	ARG
1	A	759	GLN
1	A	762	SER
1	A	765	VAL
1	A	790	ASN
1	A	852	GLN
1	A	857	LYS
1	A	858	LEU
1	A	864	LYS
1	A	866	VAL
1	A	872	SER
1	A	890	LEU
1	A	898	ASP
1	A	902	GLU
1	A	907	ASN
1	A	910	MET
1	A	916	THR
1	A	921	ILE
1	A	923	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	928	ARG
1	A	936	LYS
1	A	949	PHE
1	A	966	LEU
1	A	969	GLU
1	A	984	THR
1	A	985	THR
1	A	990	GLN
1	A	992	LEU
1	A	1000	LEU
1	A	1006	VAL
1	A	1013	VAL
1	A	1015	GLN
1	A	1027	SER
1	A	1041	THR
1	A	1045	GLU
1	A	1052	LEU
1	A	1067	LYS
1	A	1069	GLU
1	A	1071	SER
1	A	1081	LYS
1	A	1093	LEU
1	A	1122	ARG
1	A	1123	GLU
1	A	1125	THR
1	A	1129	LEU
1	A	1130	ILE
1	A	1139	ILE
2	B	97	THR
2	B	101	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	22	HIS
1	A	30	ASN
1	A	85	ASN
1	A	93	GLN
1	A	156	ASN
1	A	163	HIS
1	A	234	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	241	ASN
1	A	262	ASN
1	A	319	ASN
1	A	343	GLN
1	A	355	ASN
1	A	392	ASN
1	A	600	HIS
1	A	634	GLN
1	A	731	GLN
1	A	796	GLN
1	A	810	ASN
1	A	826	ASN
1	A	1009	HIS
1	A	1034	ASN
1	A	1055	GLN
1	A	1070	HIS
1	A	1106	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 carbohydrates 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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1114/1143 (97%)	0.02	58 (5%)	27 23	13, 59, 140, 195	0
2	B	14/14 (100%)	-0.15	1 (7%)	16 12	24, 41, 89, 91	0
All	All	1128/1157 (97%)	0.01	59 (5%)	27 23	13, 59, 140, 195	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	569	LEU	8.3
1	A	508	VAL	7.9
1	A	483	PRO	7.2
1	A	503	CYS	6.9
1	A	571	LEU	5.7
1	A	462	ASN	5.2
1	A	616	LEU	5.2
1	A	506	SER	4.6
1	A	660	TYR	4.5
1	A	556	CYS	4.3
1	A	436	LEU	4.2
1	A	460	CYS	4.0
1	A	773	SER	3.9
1	A	621	GLY	3.8
1	A	519	LEU	3.8
1	A	502	SER	3.8
1	A	507	GLN	3.7
1	A	907	ASN	3.4
1	A	294	THR	3.4
1	A	622	LEU	3.4
1	A	450	GLY	3.4
1	A	468	LEU	3.3
1	A	444	GLU	3.2
1	A	570	LYS	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	555	LEU	3.0
1	A	369	ARG	3.0
1	A	599	SER	2.9
1	A	415	SER	2.9
1	A	597	GLU	2.9
1	A	918	GLY	2.8
1	A	419	ARG	2.8
1	A	531	HIS	2.7
1	A	418	ASN	2.7
1	A	504	ASN	2.7
1	A	1015	GLN	2.7
1	A	517	TYR	2.7
1	A	568	ILE	2.6
1	A	661	SER	2.6
1	A	641	PHE	2.5
1	A	405	PRO	2.5
1	A	618	ILE	2.5
1	A	545	PRO	2.5
1	A	550	ASN	2.4
1	A	528	GLN	2.4
1	A	416	ASP	2.4
2	B	101	SER	2.3
1	A	839	GLU	2.3
1	A	486	LEU	2.3
1	A	518	TYR	2.3
1	A	602	LEU	2.2
1	A	783	GLY	2.2
1	A	1026	GLY	2.2
1	A	290	GLN	2.2
1	A	406	GLY	2.2
1	A	404	LEU	2.2
1	A	662	SER	2.1
1	A	601	TYR	2.1
1	A	467	GLN	2.1
1	A	439	ASN	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.