



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:20 AM UTC

PDB ID : 2QJ0 / pdb_00002qj0
Title : Structure of the yeast U-box-containing ubiquitin ligase Ufd2p
Authors : Tu, D.; Brunger, A.T.
Deposited on : 2007-07-06
Resolution : 2.65 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
Mogul : 2022.3.0, CSD as543be (2022)
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

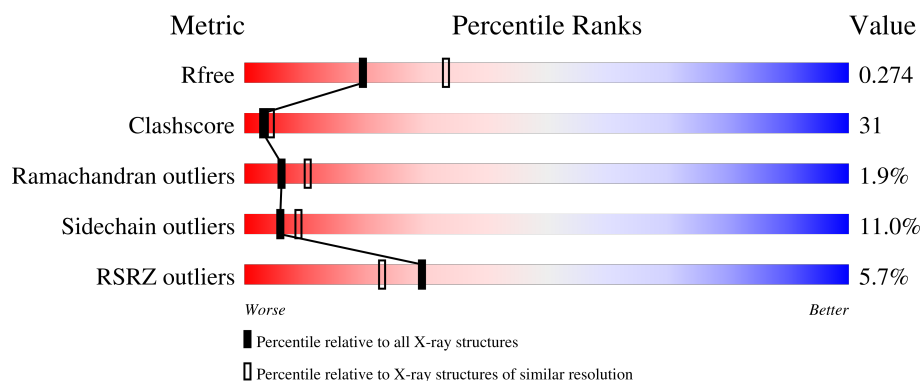
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	982	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7661 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 Ubiquitin conjugation factor E4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	937	Total	C	N	O	S	Se	0	0	0
			7567	4867	1247	1425	10	18			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	GLY	-	expression tag	UNP P54860
A	-19	SER	-	expression tag	UNP P54860
A	-18	HIS	-	expression tag	UNP P54860
A	-17	MSE	-	expression tag	UNP P54860
A	-16	ALA	-	expression tag	UNP P54860
A	-15	SER	-	expression tag	UNP P54860
A	-14	MSE	-	expression tag	UNP P54860
A	-13	THR	-	expression tag	UNP P54860
A	-12	GLY	-	expression tag	UNP P54860
A	-11	GLY	-	expression tag	UNP P54860
A	-10	GLN	-	expression tag	UNP P54860
A	-9	GLN	-	expression tag	UNP P54860
A	-8	MSE	-	expression tag	UNP P54860
A	-7	GLY	-	expression tag	UNP P54860
A	-6	ARG	-	expression tag	UNP P54860
A	-5	GLY	-	expression tag	UNP P54860
A	-4	SER	-	expression tag	UNP P54860
A	-3	GLU	-	expression tag	UNP P54860
A	-2	PHE	-	expression tag	UNP P54860
A	-1	ARG	-	expression tag	UNP P54860
A	0	SER	-	expression tag	UNP P54860
A	1	MSE	MET	modified residue	UNP P54860
A	102	LEU	SER	engineered mutation	UNP P54860
A	109	MSE	MET	modified residue	UNP P54860
A	248	MSE	MET	modified residue	UNP P54860
A	282	MSE	MET	modified residue	UNP P54860
A	312	MSE	MET	modified residue	UNP P54860

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	407	MSE	MET	modified residue	UNP P54860
A	442	MSE	MET	modified residue	UNP P54860
A	564	MSE	MET	modified residue	UNP P54860
A	590	MSE	MET	modified residue	UNP P54860
A	600	MSE	MET	modified residue	UNP P54860
A	601	MSE	MET	modified residue	UNP P54860
A	677	VAL	ASP	engineered mutation	UNP P54860
A	680	MSE	MET	modified residue	UNP P54860
A	745	MSE	MET	modified residue	UNP P54860
A	771	MSE	MET	modified residue	UNP P54860
A	890	MSE	MET	modified residue	UNP P54860
A	894	MSE	MET	modified residue	UNP P54860
A	905	MSE	MET	modified residue	UNP P54860
A	927	MSE	MET	modified residue	UNP P54860

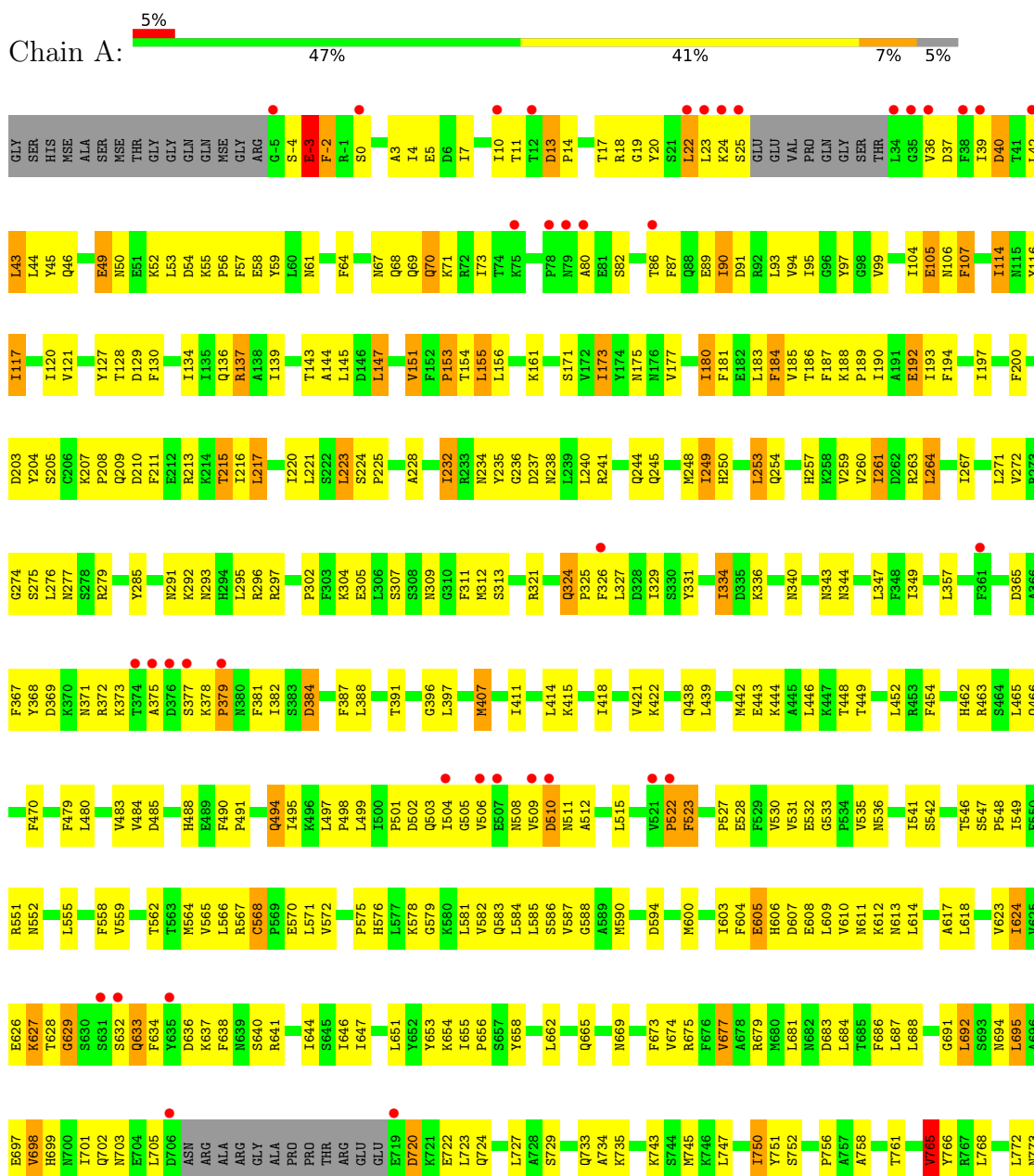
- Molecule 2 is water.

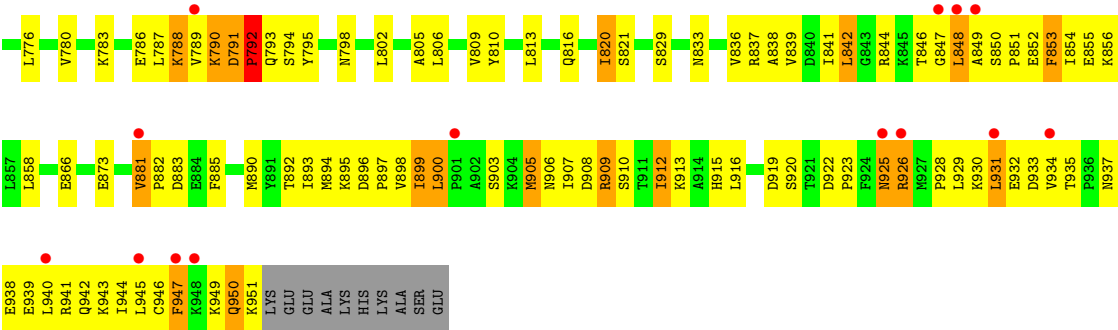
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	94	Total O 94 94	0	0

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: Ubiquitin conjugation factor E4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.80Å 122.80Å 178.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 50.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	87.4 (50.00-2.65) 84.3 (50.00-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.269 0.238 , 0.274	Depositor DCC
R_{free} test set	7381 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7661	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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	0.49	0/7709	1.04	50/10390 (0.5%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	ILE	N-CA-C	-12.56	98.04	110.72
1	A	633	GLN	N-CA-C	-12.35	94.64	111.55
1	A	629	GLY	N-CA-C	-9.47	101.69	112.29
1	A	842	LEU	N-CA-C	-9.37	101.55	113.72
1	A	-3	GLU	N-CA-C	-8.22	103.36	113.15
1	A	384	ASP	N-CA-C	-8.10	102.53	111.36
1	A	407	MSE	N-CA-C	7.75	119.72	111.28
1	A	765	VAL	N-CA-C	7.47	118.21	110.36
1	A	37	ASP	N-CA-C	-7.45	104.08	113.02
1	A	205	SER	N-CA-C	-7.23	103.46	114.16
1	A	654	LYS	N-CA-C	7.09	122.10	113.17
1	A	853	PHE	N-CA-C	-6.59	101.48	111.56
1	A	40	ASP	N-CA-C	-6.56	103.97	112.23
1	A	691	GLY	N-CA-C	-6.42	105.03	112.73
1	A	568	CYS	CA-C-N	6.33	127.75	119.84
1	A	568	CYS	C-N-CA	6.33	127.75	119.84
1	A	324	GLN	CA-C-N	6.19	125.41	118.97
1	A	324	GLN	C-N-CA	6.19	125.41	118.97
1	A	606	HIS	N-CA-C	6.16	120.95	113.38
1	A	224	SER	N-CA-C	6.14	113.65	108.13
1	A	161	LYS	N-CA-C	6.05	120.73	113.23
1	A	90	ILE	N-CA-C	-5.88	104.89	110.42
1	A	216	ILE	N-CA-C	5.88	116.34	110.23
1	A	829	SER	N-CA-C	5.88	121.42	112.54
1	A	69	GLN	N-CA-C	-5.87	106.66	113.88
1	A	145	LEU	N-CA-C	-5.87	104.88	111.28
1	A	594	ASP	N-CA-C	-5.78	106.09	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	PRO	N-CA-C	-5.71	105.94	113.65
1	A	576	HIS	N-CA-C	-5.65	105.20	111.36
1	A	624	ILE	N-CA-C	5.64	118.10	111.05
1	A	82	SER	N-CA-C	-5.62	106.39	113.20
1	A	883	ASP	N-CA-C	5.52	118.81	111.75
1	A	899	ILE	N-CA-C	5.49	116.29	107.73
1	A	925	ASN	N-CA-C	-5.38	99.00	108.20
1	A	750	ILE	N-CA-C	5.35	115.98	110.36
1	A	-2	PHE	N-CA-C	-5.35	105.57	112.68
1	A	329	ILE	N-CA-C	5.31	120.39	109.34
1	A	302	PRO	N-CA-C	-5.31	105.32	112.48
1	A	70	GLN	N-CA-C	-5.30	105.62	111.71
1	A	720	ASP	N-CA-C	5.28	120.03	111.37
1	A	173	ILE	N-CA-C	5.25	115.46	110.42
1	A	605	GLU	N-CA-C	5.23	116.79	111.14
1	A	900	LEU	N-CA-C	-5.22	102.58	109.84
1	A	144	ALA	N-CA-C	-5.20	108.70	114.62
1	A	523	PHE	N-CA-C	5.04	117.42	111.33
1	A	106	ASN	N-CA-C	5.03	115.63	108.54
1	A	236	GLY	CA-C-N	5.02	127.31	120.54
1	A	236	GLY	C-N-CA	5.02	127.31	120.54
1	A	838	ALA	N-CA-C	-5.01	105.92	112.23
1	A	947	PHE	N-CA-C	-5.00	104.90	111.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7567	0	7560	476	0
2	A	94	0	0	12	0
All	All	7661	0	7560	476	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 31.

All (476) 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:114:ILE:H	1:A:114:ILE:HD12	1.10	1.13
1:A:575:PRO:HG3	1:A:628:THR:HG21	1.22	1.10
1:A:848:LEU:HD23	1:A:848:LEU:H	1.24	1.02
1:A:14:PRO:HA	1:A:22:LEU:HD21	1.45	0.99
1:A:745:MSE:HE1	1:A:806:LEU:HD13	1.41	0.98
1:A:850:SER:HB2	1:A:851:PRO:HA	1.44	0.97
1:A:494:GLN:HE21	1:A:495:ILE:H	1.03	0.96
1:A:347:LEU:HD11	1:A:377:SER:HA	1.45	0.94
1:A:7:ILE:HD11	1:A:70:GLN:HG3	1.50	0.93
1:A:946:CYS:O	1:A:950:GLN:HB2	1.69	0.93
1:A:896:ASP:HB3	1:A:909:ARG:HB2	1.50	0.92
1:A:494:GLN:NE2	1:A:495:ILE:H	1.68	0.91
1:A:839:VAL:HG21	1:A:858:LEU:HD11	1.51	0.90
1:A:702:GLN:HG3	1:A:790:LYS:HE2	1.55	0.89
1:A:209:GLN:HG2	1:A:304:LYS:O	1.72	0.89
1:A:293:ASN:HD21	1:A:307:SER:H	1.20	0.89
1:A:701:ILE:HG21	1:A:727:LEU:HB2	1.56	0.88
1:A:207:LYS:HB3	1:A:209:GLN:HE22	1.37	0.88
1:A:114:ILE:H	1:A:114:ILE:CD1	1.84	0.86
1:A:421:VAL:HG21	1:A:442:MSE:HE1	1.55	0.85
1:A:494:GLN:HE21	1:A:495:ILE:N	1.73	0.85
1:A:695:LEU:HD13	1:A:734:ALA:HB1	1.59	0.84
1:A:261:ILE:HD11	1:A:321:ARG:NH2	1.93	0.83
1:A:117:ILE:HD13	1:A:155:LEU:HD22	1.61	0.82
1:A:375:ALA:HB3	1:A:378:LYS:HE3	1.62	0.82
1:A:117:ILE:HG12	1:A:154:THR:CG2	2.08	0.82
1:A:307:SER:HB3	1:A:312:MSE:HE1	1.62	0.81
1:A:114:ILE:HD12	1:A:114:ILE:N	1.93	0.81
1:A:848:LEU:C	1:A:850:SER:H	1.90	0.80
1:A:220:ILE:HA	1:A:223:LEU:HD22	1.64	0.80
1:A:695:LEU:HG	1:A:789:VAL:HG11	1.64	0.80
1:A:899:ILE:HD11	1:A:937:ASN:HD22	1.46	0.80
1:A:624:ILE:HG23	1:A:627:LYS:HE2	1.63	0.80
1:A:697:GLU:C	1:A:699:HIS:H	1.90	0.78
1:A:407:MSE:HE1	1:A:452:LEU:HB3	1.67	0.78
1:A:626:GLU:HB2	1:A:641:ARG:HH22	1.49	0.78
1:A:665:GLN:NE2	1:A:669:ASN:HD22	1.83	0.77
1:A:894:MSE:HE3	1:A:908:ASP:N	2.00	0.76
1:A:692:LEU:HD23	1:A:787:LEU:HD22	1.68	0.76
1:A:369:ASP:O	1:A:372:ARG:HG3	1.84	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:LEU:HD12	1:A:724:GLN:HE22	1.50	0.75
1:A:506:VAL:HG11	1:A:675:ARG:HH11	1.52	0.75
1:A:903:SER:HB3	1:A:925:ASN:ND2	2.02	0.75
1:A:930:LYS:HB2	1:A:932:GLU:HG2	1.68	0.74
1:A:900:LEU:HD21	1:A:912:ILE:HG21	1.69	0.74
1:A:841:ILE:HA	1:A:844:ARG:HD3	1.70	0.74
1:A:307:SER:CB	1:A:312:MSE:HE1	2.18	0.73
1:A:567:ARG:HG3	1:A:613:ASN:HB3	1.68	0.73
1:A:848:LEU:O	1:A:850:SER:N	2.20	0.73
1:A:64:PHE:HB2	1:A:94:VAL:HG11	1.69	0.73
1:A:326:PHE:CE2	1:A:382:ILE:HG23	2.23	0.73
1:A:117:ILE:HG12	1:A:154:THR:HG22	1.67	0.73
1:A:180:ILE:HD12	1:A:180:ILE:O	1.89	0.72
1:A:673:PHE:O	1:A:677:VAL:HG12	1.89	0.72
1:A:382:ILE:HD12	1:A:382:ILE:H	1.55	0.71
1:A:898:VAL:HG21	1:A:912:ILE:HD11	1.72	0.71
1:A:43:LEU:HD23	1:A:97:TYR:HD2	1.55	0.71
1:A:720:ASP:HA	1:A:723:LEU:HB3	1.72	0.71
1:A:905:MSE:HE2	1:A:905:MSE:HA	1.72	0.71
1:A:234:ASN:ND2	1:A:253:LEU:HD21	2.04	0.71
1:A:506:VAL:HG11	1:A:675:ARG:NH1	2.04	0.71
1:A:894:MSE:CE	1:A:897:PRO:HA	2.21	0.71
1:A:7:ILE:HG21	1:A:90:ILE:HD13	1.72	0.71
1:A:70:GLN:HB3	1:A:87:PHE:CZ	2.26	0.70
1:A:326:PHE:CZ	1:A:382:ILE:HG23	2.26	0.70
1:A:850:SER:HB2	1:A:851:PRO:CA	2.21	0.70
1:A:899:ILE:HD11	1:A:937:ASN:ND2	2.06	0.70
1:A:916:LEU:HA	1:A:919:ASP:O	1.92	0.69
1:A:752:SER:O	1:A:756:PRO:HG3	1.92	0.69
1:A:894:MSE:HE3	1:A:907:ILE:C	2.17	0.69
1:A:207:LYS:HB3	1:A:209:GLN:NE2	2.08	0.69
1:A:565:VAL:HG13	1:A:572:VAL:HG12	1.75	0.69
1:A:171:SER:O	1:A:175:ASN:HB2	1.93	0.69
1:A:357:LEU:HD23	1:A:523:PHE:CE1	2.27	0.68
1:A:220:ILE:HA	1:A:223:LEU:CD2	2.24	0.68
1:A:724:GLN:HE21	1:A:724:GLN:N	1.91	0.68
1:A:43:LEU:HD23	1:A:97:TYR:CD2	2.28	0.68
1:A:10:ILE:HD13	1:A:42:LEU:HD22	1.75	0.67
1:A:235:TYR:OH	1:A:250:HIS:HD2	1.77	0.67
1:A:839:VAL:HG13	1:A:854:ILE:HD13	1.76	0.67
1:A:261:ILE:HD11	1:A:321:ARG:CZ	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:SER:HB3	1:A:312:MSE:CE	2.23	0.67
1:A:311:PHE:HD2	1:A:312:MSE:HE1	1.59	0.67
1:A:745:MSE:CE	1:A:806:LEU:HD13	2.22	0.67
1:A:39:ILE:HD11	1:A:89:GLU:CG	2.25	0.67
1:A:99:VAL:CG2	1:A:134:ILE:HG23	2.25	0.67
1:A:215:THR:HG21	1:A:285:TYR:OH	1.95	0.66
1:A:276:LEU:HA	1:A:279:ARG:NH1	2.11	0.66
1:A:187:PHE:HB2	1:A:190:ILE:HD13	1.76	0.66
1:A:572:VAL:O	1:A:578:LYS:HE2	1.95	0.66
1:A:903:SER:HB3	1:A:925:ASN:HD22	1.61	0.66
1:A:147:LEU:O	1:A:151:VAL:HG12	1.96	0.65
1:A:632:SER:C	1:A:634:PHE:H	2.04	0.65
1:A:17:THR:HG22	1:A:17:THR:O	1.93	0.65
1:A:24:LYS:O	1:A:25:SER:HB2	1.96	0.65
1:A:894:MSE:HE2	1:A:897:PRO:HA	1.79	0.65
1:A:922:ASP:HB3	1:A:925:ASN:O	1.97	0.65
1:A:307:SER:CB	1:A:312:MSE:CE	2.75	0.65
1:A:702:GLN:HG3	1:A:790:LYS:CE	2.26	0.64
1:A:71:LYS:HG2	1:A:87:PHE:HD2	1.62	0.64
1:A:503:GLN:HB3	1:A:506:VAL:CA	2.28	0.64
1:A:839:VAL:HG21	1:A:858:LEU:CD1	2.26	0.64
1:A:898:VAL:HG11	1:A:909:ARG:HG2	1.80	0.64
1:A:130:PHE:O	1:A:134:ILE:HG13	1.98	0.63
1:A:414:LEU:O	1:A:418:ILE:HG23	1.98	0.63
1:A:897:PRO:HD2	1:A:941:ARG:HD3	1.79	0.63
1:A:439:LEU:HA	1:A:442:MSE:HE3	1.80	0.63
1:A:905:MSE:HA	1:A:905:MSE:CE	2.28	0.63
1:A:816:GLN:O	1:A:820:ILE:HG23	1.99	0.63
1:A:173:ILE:HD12	1:A:173:ILE:H	1.64	0.63
1:A:729:SER:O	1:A:733:GLN:HG3	1.98	0.62
1:A:750:ILE:HG22	1:A:751:TYR:HD1	1.64	0.62
1:A:188:LYS:O	1:A:192:GLU:HG2	2.00	0.62
1:A:117:ILE:O	1:A:121:VAL:HG23	2.00	0.62
1:A:187:PHE:CB	1:A:190:ILE:HD13	2.30	0.62
1:A:117:ILE:HG12	1:A:154:THR:HG21	1.79	0.62
1:A:297:ARG:CG	1:A:297:ARG:HH11	2.13	0.62
1:A:941:ARG:HA	1:A:944:ILE:HD12	1.81	0.62
1:A:99:VAL:HG22	1:A:134:ILE:HG23	1.82	0.62
1:A:502:ASP:CG	1:A:567:ARG:HH12	2.08	0.62
1:A:326:PHE:HB2	1:A:327:LEU:HD13	1.82	0.61
1:A:851:PRO:O	1:A:855:GLU:HB2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:PRO:CA	1:A:22:LEU:HD21	2.26	0.61
1:A:503:GLN:HB3	1:A:506:VAL:HA	1.81	0.61
1:A:46:GLN:O	1:A:53:LEU:HD12	2.01	0.61
1:A:846:THR:HA	1:A:848:LEU:CD2	2.30	0.61
1:A:180:ILE:O	1:A:184:PHE:HB2	2.00	0.61
1:A:692:LEU:CD2	1:A:787:LEU:HD22	2.30	0.61
1:A:697:GLU:C	1:A:699:HIS:N	2.58	0.61
1:A:181:PHE:HB3	1:A:267:ILE:HD13	1.81	0.61
1:A:375:ALA:HB3	1:A:378:LYS:CE	2.31	0.60
1:A:665:GLN:HE21	1:A:669:ASN:HD22	1.46	0.60
1:A:930:LYS:O	1:A:932:GLU:N	2.34	0.60
1:A:628:THR:HG22	1:A:629:GLY:H	1.65	0.60
1:A:260:VAL:O	1:A:264:LEU:HB2	2.02	0.60
1:A:4:ILE:HD13	1:A:39:ILE:CG2	2.32	0.60
1:A:117:ILE:HD13	1:A:155:LEU:CD2	2.31	0.60
1:A:225:PRO:HB3	1:A:253:LEU:HD12	1.82	0.60
1:A:71:LYS:HG2	1:A:87:PHE:CD2	2.37	0.59
1:A:0:SER:OG	1:A:86:THR:HG21	2.02	0.59
1:A:44:LEU:HD23	1:A:44:LEU:O	2.01	0.59
1:A:848:LEU:HD23	1:A:848:LEU:N	2.06	0.59
1:A:850:SER:HA	1:A:853:PHE:H	1.66	0.59
1:A:894:MSE:HE3	1:A:908:ASP:CA	2.32	0.59
1:A:128:THR:HG23	1:A:129:ASP:H	1.68	0.59
1:A:679:ARG:NH2	1:A:683:ASP:OD1	2.35	0.58
1:A:722:GLU:O	1:A:722:GLU:HG2	2.03	0.58
1:A:724:GLN:HE21	1:A:724:GLN:CA	2.16	0.58
1:A:850:SER:HB3	1:A:854:ILE:HG13	1.83	0.58
1:A:626:GLU:HB2	1:A:641:ARG:NH2	2.17	0.58
1:A:646:ILE:HA	2:A:972:HOH:O	2.04	0.58
1:A:344:ASN:HB2	2:A:1028:HOH:O	2.03	0.58
1:A:697:GLU:O	1:A:699:HIS:N	2.36	0.58
1:A:311:PHE:HD2	1:A:312:MSE:CE	2.16	0.58
1:A:257:HIS:HA	1:A:260:VAL:CG1	2.33	0.58
1:A:842:LEU:O	1:A:848:LEU:HD22	2.02	0.58
1:A:369:ASP:C	1:A:371:ASN:H	2.11	0.58
1:A:189:PRO:O	1:A:193:ILE:HD12	2.04	0.57
1:A:509:VAL:O	1:A:510:ASP:C	2.46	0.57
1:A:50:ASN:HD21	1:A:52:LYS:HB2	1.69	0.57
1:A:367:PHE:O	1:A:371:ASN:ND2	2.37	0.57
1:A:387:PHE:O	1:A:391:THR:CG2	2.53	0.57
1:A:67:ASN:CG	1:A:90:ILE:HG21	2.30	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:VAL:HG21	1:A:912:ILE:CD1	2.35	0.57
1:A:531:VAL:O	1:A:535:VAL:HG23	2.03	0.57
1:A:-3:GLU:CD	1:A:-3:GLU:H	2.13	0.57
1:A:640:SER:O	1:A:644:ILE:HG13	2.04	0.57
1:A:312:MSE:HE2	1:A:312:MSE:N	2.19	0.56
1:A:173:ILE:HD12	1:A:173:ILE:N	2.19	0.56
1:A:-4:SER:C	1:A:-2:PHE:H	2.11	0.56
1:A:234:ASN:HB3	1:A:249:ILE:CD1	2.35	0.56
1:A:257:HIS:HA	1:A:260:VAL:HG12	1.86	0.56
1:A:945:LEU:HB3	1:A:949:LYS:HE2	1.87	0.56
1:A:349:ILE:HD13	1:A:391:THR:HG21	1.88	0.56
1:A:411:ILE:O	1:A:415:LYS:HG3	2.05	0.56
1:A:463:ARG:HG2	1:A:546:THR:HB	1.88	0.56
1:A:18:ARG:HD3	1:A:19:GLY:H	1.70	0.55
1:A:194:PHE:HB3	1:A:271:LEU:CD2	2.36	0.55
1:A:735:LYS:HA	1:A:795:TYR:O	2.06	0.55
1:A:194:PHE:O	1:A:197:ILE:HG13	2.07	0.55
1:A:816:GLN:HG2	2:A:975:HOH:O	2.05	0.55
1:A:848:LEU:C	1:A:850:SER:N	2.62	0.55
1:A:143:THR:O	1:A:143:THR:HG23	2.07	0.55
1:A:382:ILE:H	1:A:382:ILE:CD1	2.20	0.55
1:A:532:GLU:HG2	1:A:536:ASN:ND2	2.21	0.55
1:A:900:LEU:HD21	1:A:912:ILE:CG2	2.37	0.55
1:A:128:THR:HG23	1:A:129:ASP:N	2.21	0.54
1:A:698:VAL:HG12	1:A:698:VAL:O	2.05	0.54
1:A:326:PHE:CZ	1:A:382:ILE:HG13	2.43	0.54
1:A:633:GLN:HG2	1:A:636:ASP:OD2	2.08	0.54
1:A:555:LEU:HB3	1:A:603:ILE:CD1	2.37	0.54
1:A:833:ASN:O	1:A:836:VAL:HB	2.07	0.54
1:A:846:THR:HA	1:A:848:LEU:HD21	1.88	0.54
1:A:3:ALA:HA	2:A:995:HOH:O	2.08	0.54
1:A:130:PHE:CE2	1:A:134:ILE:HD11	2.43	0.54
1:A:727:LEU:HD23	1:A:727:LEU:C	2.32	0.54
1:A:462:HIS:CD2	1:A:465:LEU:HD12	2.43	0.54
1:A:7:ILE:CD1	1:A:70:GLN:HG3	2.30	0.54
1:A:208:PRO:HG2	1:A:305:GLU:O	2.09	0.54
1:A:244:GLN:O	1:A:248:MSE:HG2	2.08	0.54
1:A:906:ASN:HD22	1:A:940:LEU:HD22	1.72	0.54
1:A:894:MSE:CE	1:A:907:ILE:C	2.81	0.53
1:A:39:ILE:HD11	1:A:89:GLU:HG3	1.89	0.53
1:A:588:GLY:O	1:A:600:MSE:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ASN:HB3	1:A:515:LEU:HG	1.90	0.53
1:A:564:MSE:HE3	1:A:571:LEU:HD13	1.90	0.53
1:A:695:LEU:HD13	1:A:734:ALA:CB	2.35	0.53
1:A:565:VAL:HG13	1:A:572:VAL:CG1	2.39	0.53
1:A:906:ASN:ND2	1:A:940:LEU:HD22	2.23	0.53
1:A:855:GLU:OE1	1:A:855:GLU:HA	2.09	0.53
1:A:898:VAL:HB	1:A:934:VAL:CG1	2.39	0.53
1:A:930:LYS:C	1:A:932:GLU:H	2.17	0.53
1:A:568:CYS:HB3	1:A:570:GLU:OE1	2.08	0.53
1:A:411:ILE:HG23	1:A:446:LEU:HD11	1.92	0.52
1:A:220:ILE:CA	1:A:223:LEU:HD22	2.38	0.52
1:A:357:LEU:CD1	1:A:528:GLU:HA	2.40	0.52
1:A:438:GLN:HG2	1:A:442:MSE:HE2	1.91	0.52
1:A:234:ASN:HB3	1:A:249:ILE:HD12	1.92	0.52
1:A:245:GLN:O	1:A:248:MSE:HB2	2.09	0.52
1:A:448:THR:O	1:A:452:LEU:HB2	2.09	0.52
1:A:780:VAL:HG11	1:A:837:ARG:HG3	1.92	0.52
1:A:211:PHE:O	1:A:215:THR:HB	2.10	0.52
1:A:899:ILE:CD1	1:A:937:ASN:HD22	2.21	0.52
1:A:612:LYS:C	1:A:613:ASN:HD22	2.17	0.52
1:A:498:PRO:HG3	1:A:567:ARG:NH1	2.26	0.51
1:A:388:LEU:HA	1:A:391:THR:HG23	1.92	0.51
1:A:854:ILE:O	1:A:858:LEU:HD13	2.11	0.51
1:A:894:MSE:HE3	1:A:908:ASP:HA	1.91	0.51
1:A:64:PHE:HB2	1:A:94:VAL:CG1	2.40	0.51
1:A:228:ALA:O	1:A:232:ILE:HG23	2.10	0.51
1:A:261:ILE:CD1	1:A:321:ARG:CZ	2.89	0.51
1:A:444:LYS:HE2	2:A:1012:HOH:O	2.10	0.51
1:A:479:PHE:O	1:A:483:VAL:HG23	2.10	0.51
1:A:551:ARG:HG3	1:A:551:ARG:HH11	1.76	0.51
1:A:626:GLU:C	1:A:628:THR:H	2.18	0.51
1:A:312:MSE:HE2	1:A:312:MSE:CA	2.41	0.51
1:A:632:SER:C	1:A:634:PHE:N	2.68	0.51
1:A:490:PHE:CG	1:A:491:PRO:HA	2.46	0.51
1:A:776:LEU:HB2	1:A:806:LEU:HD21	1.92	0.51
1:A:375:ALA:HB3	1:A:378:LYS:CD	2.41	0.51
1:A:947:PHE:C	1:A:949:LYS:H	2.20	0.50
1:A:765:VAL:CG1	1:A:766:TYR:N	2.75	0.50
1:A:940:LEU:C	1:A:942:GLN:H	2.19	0.50
1:A:382:ILE:HD12	1:A:382:ILE:N	2.23	0.50
1:A:944:ILE:O	1:A:944:ILE:HG22	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:TYR:CZ	1:A:750:ILE:HD11	2.47	0.50
1:A:611:ASN:HA	1:A:658:TYR:OH	2.12	0.50
1:A:783:LYS:HG3	2:A:997:HOH:O	2.11	0.49
1:A:505:GLY:O	1:A:508:ASN:ND2	2.40	0.49
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.77	0.49
1:A:683:ASP:O	1:A:687:LEU:HG	2.12	0.49
1:A:99:VAL:HG23	1:A:134:ILE:HG23	1.94	0.49
1:A:307:SER:HB2	1:A:312:MSE:CE	2.42	0.49
1:A:378:LYS:N	1:A:379:PRO:CD	2.76	0.49
1:A:915:HIS:CD2	1:A:923:PRO:HG3	2.47	0.49
1:A:61:ASN:HD22	1:A:130:PHE:CB	2.26	0.49
1:A:99:VAL:HG22	1:A:134:ILE:CG2	2.41	0.49
1:A:235:TYR:OH	1:A:250:HIS:CD2	2.61	0.49
1:A:758:ALA:O	1:A:761:THR:HG22	2.13	0.49
1:A:848:LEU:H	1:A:848:LEU:CD2	2.05	0.49
1:A:852:GLU:O	1:A:856:LYS:HG3	2.13	0.49
1:A:297:ARG:CG	1:A:297:ARG:NH1	2.74	0.49
1:A:439:LEU:O	1:A:443:GLU:HG2	2.13	0.49
1:A:945:LEU:C	1:A:947:PHE:H	2.21	0.49
1:A:91:ASP:O	1:A:95:ILE:HG12	2.13	0.48
1:A:624:ILE:O	1:A:627:LYS:HG2	2.12	0.48
1:A:155:LEU:CD1	1:A:177:VAL:HG13	2.43	0.48
1:A:200:PHE:CE2	1:A:217:LEU:CD2	2.95	0.48
1:A:651:LEU:HD22	1:A:658:TYR:CD1	2.48	0.48
1:A:780:VAL:HG12	1:A:780:VAL:O	2.13	0.48
1:A:503:GLN:O	1:A:506:VAL:HB	2.13	0.48
1:A:895:LYS:O	1:A:941:ARG:HD3	2.14	0.48
1:A:36:VAL:CG2	1:A:86:THR:HG22	2.43	0.48
1:A:567:ARG:CG	1:A:613:ASN:HB3	2.42	0.48
1:A:237:ASP:OD2	1:A:241:ARG:NH2	2.46	0.48
1:A:618:LEU:HD11	1:A:647:ILE:HG21	1.96	0.48
1:A:331:TYR:CD1	1:A:334:ILE:HD12	2.48	0.48
1:A:387:PHE:O	1:A:391:THR:HG22	2.13	0.48
1:A:511:ASN:O	1:A:512:ALA:C	2.57	0.48
1:A:930:LYS:C	1:A:932:GLU:N	2.72	0.48
1:A:387:PHE:O	1:A:391:THR:HG23	2.14	0.48
1:A:765:VAL:HG13	1:A:766:TYR:N	2.28	0.48
1:A:950:GLN:O	1:A:951:LYS:C	2.57	0.48
1:A:583:GLN:O	1:A:587:VAL:HG23	2.14	0.47
1:A:628:THR:CG2	1:A:629:GLY:H	2.24	0.47
1:A:655:ILE:O	1:A:656:PRO:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:HG3	1:A:551:ARG:NH1	2.28	0.47
1:A:572:VAL:HG13	1:A:578:LYS:HE2	1.96	0.47
1:A:331:TYR:HD1	1:A:334:ILE:HD12	1.79	0.47
1:A:357:LEU:HD13	1:A:528:GLU:HA	1.95	0.47
1:A:533:GLY:HA3	2:A:976:HOH:O	2.14	0.47
1:A:695:LEU:HG	1:A:789:VAL:CG1	2.42	0.47
1:A:153:PRO:O	1:A:156:LEU:HB3	2.14	0.47
1:A:293:ASN:HD21	1:A:307:SER:N	2.01	0.47
1:A:614:LEU:HD13	1:A:651:LEU:HD11	1.97	0.47
1:A:780:VAL:O	1:A:837:ARG:NH2	2.47	0.47
1:A:847:GLY:N	1:A:848:LEU:HD23	2.29	0.47
1:A:259:VAL:O	1:A:263:ARG:HG3	2.15	0.47
1:A:291:ASN:C	1:A:292:LYS:HD2	2.40	0.47
1:A:297:ARG:NH1	1:A:297:ARG:HG3	2.30	0.47
1:A:905:MSE:CE	2:A:1009:HOH:O	2.63	0.47
1:A:945:LEU:C	1:A:947:PHE:N	2.72	0.47
1:A:735:LYS:HB2	1:A:795:TYR:HA	1.96	0.47
1:A:820:ILE:HD12	1:A:820:ILE:C	2.39	0.47
1:A:566:LEU:O	1:A:617:ALA:HB1	2.14	0.47
1:A:612:LYS:C	1:A:613:ASN:ND2	2.74	0.47
1:A:116:TYR:O	1:A:120:ILE:HG13	2.15	0.46
1:A:411:ILE:HG22	1:A:415:LYS:HD2	1.97	0.46
1:A:940:LEU:C	1:A:942:GLN:N	2.72	0.46
1:A:694:ASN:O	1:A:698:VAL:HG23	2.15	0.46
1:A:365:ASP:O	1:A:368:TYR:HB2	2.15	0.46
1:A:497:LEU:HD22	1:A:609:LEU:HD11	1.97	0.46
1:A:558:PHE:HE2	1:A:584:LEU:CD2	2.28	0.46
1:A:562:THR:HG21	1:A:585:LEU:HD13	1.98	0.46
1:A:820:ILE:HG13	1:A:821:SER:N	2.30	0.46
1:A:522:PRO:HG2	1:A:523:PHE:H	1.80	0.46
1:A:745:MSE:HE3	1:A:806:LEU:HB2	1.96	0.46
1:A:896:ASP:OD1	1:A:909:ARG:HG3	2.15	0.46
1:A:940:LEU:O	1:A:944:ILE:HG13	2.16	0.46
1:A:527:PRO:HG2	1:A:530:VAL:HG23	1.97	0.46
1:A:653:TYR:OH	1:A:750:ILE:HD11	2.16	0.46
1:A:833:ASN:HD22	1:A:836:VAL:HB	1.80	0.46
1:A:250:HIS:O	1:A:254:GLN:HG3	2.15	0.46
1:A:588:GLY:HA3	1:A:600:MSE:HB2	1.97	0.46
1:A:773:ASN:ND2	1:A:810:TYR:OH	2.48	0.46
1:A:422:LYS:HG3	1:A:439:LEU:HD11	1.97	0.46
1:A:791:ASP:O	1:A:794:SER:OG	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PHE:CD1	1:A:491:PRO:HA	2.51	0.46
1:A:628:THR:HG22	1:A:629:GLY:N	2.28	0.46
1:A:50:ASN:ND2	1:A:52:LYS:H	2.14	0.46
1:A:155:LEU:HD22	1:A:155:LEU:HA	1.72	0.46
1:A:104:ILE:O	1:A:105:GLU:C	2.60	0.45
1:A:498:PRO:HG3	1:A:567:ARG:CZ	2.46	0.45
1:A:937:ASN:OD1	1:A:940:LEU:HB2	2.16	0.45
1:A:89:GLU:OE1	1:A:89:GLU:HA	2.16	0.45
1:A:186:THR:O	1:A:186:THR:HG22	2.16	0.45
1:A:204:TYR:CG	1:A:204:TYR:O	2.68	0.45
1:A:494:GLN:HE21	1:A:494:GLN:CA	2.29	0.45
1:A:336:LYS:HB3	1:A:382:ILE:HG21	1.98	0.45
1:A:497:LEU:HD12	1:A:499:LEU:CD2	2.45	0.45
1:A:885:PHE:O	1:A:893:ILE:HD12	2.17	0.45
1:A:898:VAL:HG22	1:A:907:ILE:O	2.16	0.45
1:A:900:LEU:HD13	1:A:922:ASP:OD1	2.17	0.45
1:A:-4:SER:C	1:A:-2:PHE:N	2.74	0.45
1:A:745:MSE:HG3	1:A:802:LEU:HD11	1.99	0.45
1:A:194:PHE:HB3	1:A:271:LEU:HD21	1.99	0.45
1:A:786:GLU:O	1:A:788:LYS:HD3	2.17	0.45
1:A:-2:PHE:C	1:A:0:SER:N	2.72	0.45
1:A:220:ILE:O	1:A:223:LEU:HD22	2.16	0.45
1:A:238:ASN:ND2	1:A:240:LEU:H	2.14	0.45
1:A:309:ASN:O	1:A:313:SER:HB2	2.17	0.45
1:A:407:MSE:HE2	1:A:449:THR:HG23	1.99	0.45
1:A:852:GLU:H	1:A:852:GLU:HG3	1.50	0.45
1:A:894:MSE:HE1	1:A:897:PRO:HA	1.96	0.45
1:A:909:ARG:HG3	1:A:909:ARG:HH11	1.82	0.45
1:A:36:VAL:O	1:A:39:ILE:HG12	2.17	0.45
1:A:637:LYS:HE3	1:A:638:PHE:CZ	2.51	0.45
1:A:805:ALA:O	1:A:809:VAL:HG23	2.17	0.45
1:A:938:GLU:O	1:A:939:GLU:C	2.59	0.45
1:A:10:ILE:HD11	1:A:23:LEU:HB3	1.98	0.45
1:A:95:ILE:HD11	1:A:137:ARG:NH1	2.32	0.45
1:A:56:PRO:O	1:A:59:TYR:HB3	2.17	0.44
1:A:532:GLU:HG2	1:A:536:ASN:HD21	1.81	0.44
1:A:572:VAL:O	1:A:572:VAL:HG13	2.15	0.44
1:A:235:TYR:C	1:A:237:ASP:H	2.24	0.44
1:A:36:VAL:CG1	1:A:86:THR:HG22	2.47	0.44
1:A:95:ILE:HA	1:A:130:PHE:HE1	1.82	0.44
1:A:662:LEU:HD21	1:A:751:TYR:CD2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASP:C	1:A:371:ASN:N	2.72	0.44
1:A:555:LEU:HD22	1:A:559:VAL:HG23	1.98	0.44
1:A:248:MSE:HA	1:A:248:MSE:HE2	1.99	0.44
1:A:583:GLN:O	1:A:586:SER:OG	2.33	0.44
1:A:604:PHE:HA	1:A:610:VAL:HG11	2.00	0.44
1:A:674:VAL:HA	1:A:677:VAL:HG13	1.99	0.44
1:A:324:GLN:HB3	1:A:325:PRO:HD3	2.00	0.44
1:A:117:ILE:HA	1:A:120:ILE:HD12	2.00	0.44
1:A:858:LEU:HD12	1:A:858:LEU:N	2.31	0.44
1:A:912:ILE:HG13	1:A:913:LYS:H	1.82	0.44
1:A:67:ASN:OD1	1:A:90:ILE:HD12	2.18	0.43
1:A:541:ILE:HD12	1:A:542:SER:N	2.33	0.43
1:A:17:THR:O	1:A:17:THR:CG2	2.64	0.43
1:A:791:ASP:O	1:A:792:PRO:C	2.61	0.43
1:A:274:GLY:O	1:A:275:SER:HB3	2.18	0.43
1:A:586:SER:O	1:A:590:MSE:HG2	2.19	0.43
1:A:217:LEU:HB3	1:A:221:LEU:CD1	2.48	0.43
1:A:235:TYR:C	1:A:237:ASP:N	2.75	0.43
1:A:905:MSE:HE2	2:A:1009:HOH:O	2.18	0.43
1:A:293:ASN:HD22	1:A:296:ARG:HG3	1.84	0.43
1:A:920:SER:O	1:A:928:PRO:HA	2.18	0.43
1:A:907:ILE:HD13	1:A:912:ILE:HG23	2.00	0.43
1:A:909:ARG:O	1:A:913:LYS:HB2	2.18	0.43
1:A:261:ILE:HA	1:A:264:LEU:HB2	2.00	0.43
1:A:559:VAL:HG12	1:A:610:VAL:HG21	2.01	0.43
1:A:607:ASP:O	1:A:608:GLU:C	2.61	0.43
1:A:688:LEU:O	1:A:692:LEU:HB2	2.19	0.43
1:A:20:TYR:N	1:A:20:TYR:CD1	2.87	0.43
1:A:136:GLN:O	1:A:139:ILE:HG12	2.19	0.43
1:A:497:LEU:HD12	1:A:499:LEU:HD21	2.00	0.43
1:A:590:MSE:HE2	1:A:590:MSE:HA	2.00	0.43
1:A:925:ASN:O	1:A:925:ASN:CG	2.62	0.43
1:A:55:LYS:HD3	1:A:58:GLU:OE1	2.17	0.42
1:A:340:ASN:HB3	1:A:343:ASN:CG	2.44	0.42
1:A:40:ASP:HA	1:A:93:LEU:HD13	2.00	0.42
1:A:548:PRO:O	1:A:552:ASN:HB2	2.18	0.42
1:A:183:LEU:HD13	1:A:183:LEU:C	2.44	0.42
1:A:683:ASP:HA	1:A:686:PHE:CE2	2.54	0.42
1:A:780:VAL:HG12	1:A:837:ARG:HE	1.85	0.42
1:A:950:GLN:HB3	1:A:951:LYS:H	1.67	0.42
1:A:541:ILE:HD11	1:A:549:ILE:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG21	1:A:86:THR:HG22	2.01	0.42
1:A:897:PRO:HG3	1:A:941:ARG:HB2	2.01	0.42
1:A:909:ARG:O	1:A:912:ILE:HG13	2.20	0.42
1:A:18:ARG:HG3	1:A:20:TYR:CE1	2.55	0.42
1:A:71:LYS:C	1:A:73:ILE:H	2.27	0.42
1:A:210:ASP:OD1	1:A:213:ARG:NH1	2.53	0.42
1:A:890:MSE:O	1:A:892:THR:HG23	2.20	0.42
1:A:234:ASN:HB3	1:A:249:ILE:HD11	2.02	0.42
1:A:384:ASP:O	1:A:388:LEU:HB2	2.20	0.42
1:A:768:LEU:O	1:A:772:LEU:HG	2.20	0.42
1:A:107:PHE:CD1	1:A:107:PHE:C	2.97	0.42
1:A:155:LEU:HD11	1:A:177:VAL:HG13	2.02	0.42
1:A:470:PHE:CE2	1:A:549:ILE:HA	2.55	0.42
1:A:503:GLN:HB3	1:A:506:VAL:HB	2.01	0.42
1:A:756:PRO:HB3	1:A:813:LEU:HD23	2.02	0.42
1:A:909:ARG:HE	1:A:931:LEU:HD11	1.84	0.42
1:A:36:VAL:HG21	1:A:86:THR:CG2	2.49	0.41
1:A:947:PHE:C	1:A:949:LYS:N	2.76	0.41
1:A:13:ASP:O	1:A:13:ASP:CG	2.63	0.41
1:A:57:PHE:HE2	1:A:127:TYR:HD1	1.68	0.41
1:A:13:ASP:O	1:A:13:ASP:OD1	2.38	0.41
1:A:36:VAL:O	1:A:36:VAL:HG12	2.21	0.41
1:A:129:ASP:HB2	2:A:1005:HOH:O	2.21	0.41
1:A:221:LEU:HD23	1:A:264:LEU:CD1	2.50	0.41
1:A:324:GLN:N	1:A:325:PRO:CD	2.83	0.41
1:A:480:LEU:HD11	1:A:530:VAL:CG1	2.51	0.41
1:A:484:VAL:O	1:A:485:ASP:C	2.64	0.41
1:A:899:ILE:HG22	1:A:900:LEU:O	2.21	0.41
1:A:215:THR:CG2	1:A:285:TYR:OH	2.65	0.41
1:A:703:ASN:C	1:A:705:LEU:N	2.79	0.41
1:A:235:TYR:CD1	1:A:454:PHE:HB3	2.54	0.41
1:A:381:PHE:O	1:A:382:ILE:C	2.64	0.41
1:A:890:MSE:C	1:A:892:THR:H	2.29	0.41
1:A:5:GLU:HG2	1:A:11:THR:HG22	2.02	0.41
1:A:221:LEU:HD23	1:A:264:LEU:HD11	2.02	0.41
1:A:340:ASN:HA	1:A:343:ASN:OD1	2.20	0.41
1:A:566:LEU:HD12	1:A:566:LEU:HA	1.78	0.41
1:A:839:VAL:CG2	1:A:858:LEU:HD11	2.37	0.41
1:A:312:MSE:HG2	1:A:396:GLY:HA2	2.03	0.41
1:A:546:THR:O	1:A:547:SER:C	2.63	0.41
1:A:605:GLU:HB2	1:A:655:ILE:HD13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:LEU:HD23	1:A:787:LEU:HD21	2.03	0.41
1:A:943:LYS:C	1:A:945:LEU:H	2.28	0.41
1:A:45:TYR:CD1	1:A:49:GLU:HB2	2.56	0.41
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.92	0.41
1:A:581:LEU:HA	1:A:581:LEU:HD23	1.83	0.41
1:A:626:GLU:O	1:A:628:THR:N	2.51	0.41
1:A:137:ARG:HH11	1:A:137:ARG:CG	2.34	0.40
1:A:501:PRO:HA	2:A:1022:HOH:O	2.21	0.40
1:A:623:VAL:HG11	1:A:675:ARG:HE	1.85	0.40
1:A:173:ILE:H	1:A:173:ILE:CD1	2.30	0.40
1:A:703:ASN:C	1:A:705:LEU:H	2.30	0.40
1:A:894:MSE:HE2	1:A:897:PRO:CA	2.49	0.40
1:A:466:GLN:HB3	1:A:548:PRO:HG2	2.03	0.40
1:A:848:LEU:O	1:A:848:LEU:HG	2.21	0.40
1:A:881:VAL:O	1:A:882:PRO:C	2.63	0.40
1:A:95:ILE:HA	1:A:130:PHE:CE1	2.56	0.40
1:A:194:PHE:CG	1:A:271:LEU:HD21	2.57	0.40
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.89	0.40
1:A:579:GLY:O	1:A:582:VAL:HG12	2.22	0.40
1:A:743:LYS:HE3	2:A:972:HOH:O	2.21	0.40
1:A:747:LEU:HD23	1:A:747:LEU:HA	1.92	0.40
1:A:943:LYS:HA	1:A:946:CYS:SG	2.60	0.40
1:A:209:GLN:CD	1:A:209:GLN:H	2.29	0.40
1:A:723:LEU:HD12	1:A:724:GLN:NE2	2.29	0.40
1:A:898:VAL:HB	1:A:934:VAL:HG12	2.02	0.40
1:A:932:GLU:HG3	1:A:933:ASP:N	2.36	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	931/982 (95%)	792 (85%)	121 (13%)	18 (2%)	6 10

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	849	ALA
1	A	931	LEU
1	A	950	GLN
1	A	105	GLU
1	A	494	GLN
1	A	627	LYS
1	A	698	VAL
1	A	790	LYS
1	A	373	LYS
1	A	510	ASP
1	A	522	PRO
1	A	792	PRO
1	A	379	PRO
1	A	926	ARG
1	A	80	ALA
1	A	488	HIS
1	A	866	GLU
1	A	334	ILE

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	464/861 (54%)	413 (89%)	51 (11%)	6 9

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	GLU
1	A	13	ASP
1	A	22	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	43	LEU
1	A	49	GLU
1	A	54	ASP
1	A	68	GLN
1	A	107	PHE
1	A	114	ILE
1	A	117	ILE
1	A	137	ARG
1	A	147	LEU
1	A	151	VAL
1	A	155	LEU
1	A	180	ILE
1	A	184	PHE
1	A	185	VAL
1	A	192	GLU
1	A	203	ASP
1	A	215	THR
1	A	217	LEU
1	A	223	LEU
1	A	232	ILE
1	A	249	ILE
1	A	253	LEU
1	A	261	ILE
1	A	264	LEU
1	A	272	VAL
1	A	277	ASN
1	A	677	VAL
1	A	681	LEU
1	A	684	LEU
1	A	692	LEU
1	A	695	LEU
1	A	765	VAL
1	A	788	LYS
1	A	791	ASP
1	A	792	PRO
1	A	793	GLN
1	A	798	ASN
1	A	820	ILE
1	A	848	LEU
1	A	873	GLU
1	A	881	VAL
1	A	905	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	909	ARG
1	A	910	SER
1	A	912	ILE
1	A	926	ARG
1	A	929	LEU
1	A	935	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	50	ASN
1	A	61	ASN
1	A	68	GLN
1	A	103	GLN
1	A	175	ASN
1	A	209	GLN
1	A	234	ASN
1	A	238	ASN
1	A	250	HIS
1	A	277	ASN
1	A	665	GLN
1	A	667	GLN
1	A	773	ASN
1	A	793	GLN
1	A	833	ASN
1	A	906	ASN
1	A	915	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 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	919/982 (93%)	0.34	52 (5%) 29 23	38, 71, 125, 151	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	SER	4.4
1	A	849	ALA	4.4
1	A	38	PHE	4.2
1	A	23	LEU	4.0
1	A	521	VAL	3.8
1	A	377	SER	3.7
1	A	326	PHE	3.7
1	A	522	PRO	3.6
1	A	39	ILE	3.4
1	A	504	ILE	3.4
1	A	847	GLY	3.3
1	A	42	LEU	3.0
1	A	375	ALA	2.9
1	A	948	LYS	2.9
1	A	631	SER	2.7
1	A	78	PRO	2.7
1	A	80	ALA	2.6
1	A	706	ASP	2.6
1	A	376	ASP	2.6
1	A	36	VAL	2.6
1	A	632	SER	2.5
1	A	925	ASN	2.5
1	A	506	VAL	2.4
1	A	931	LEU	2.4
1	A	635	TYR	2.4
1	A	881	VAL	2.4
1	A	10	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	-5	GLY	2.4
1	A	901	PRO	2.3
1	A	947	PHE	2.3
1	A	86	THR	2.3
1	A	926	ARG	2.3
1	A	509	VAL	2.3
1	A	24	LYS	2.3
1	A	374	THR	2.2
1	A	22	LEU	2.2
1	A	34	LEU	2.2
1	A	507	GLU	2.2
1	A	719	GLU	2.2
1	A	510	ASP	2.2
1	A	945	LEU	2.2
1	A	361	PHE	2.2
1	A	12	THR	2.1
1	A	79	ASN	2.1
1	A	940	LEU	2.1
1	A	35	GLY	2.1
1	A	789	VAL	2.1
1	A	75	LYS	2.1
1	A	379	PRO	2.1
1	A	848	LEU	2.0
1	A	0	SER	2.0
1	A	934	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.