



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:00 PM UTC

PDB ID : 7BII / pdb_00007bii
Title : Crystal structure of Nematocida HUWE1
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Deposited on : 2021-01-12
Resolution : 3.04 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

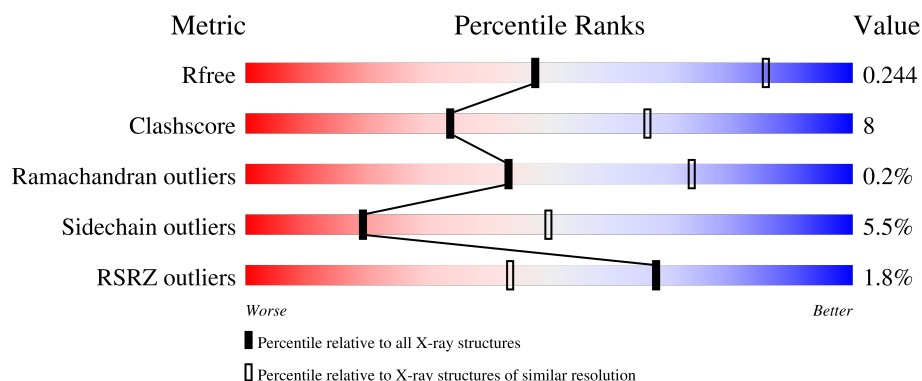
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	2492	% 67% 18% • 14%
1	B	2492	2% 67% 18% • 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34901 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 E3 ubiquitin-protein ligase HUWE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2143	Total	C	N	O	S	0	0	0
			17453	11280	2862	3213	98			
1	B	2144	Total	C	N	O	S	0	0	0
			17448	11273	2861	3216	98			

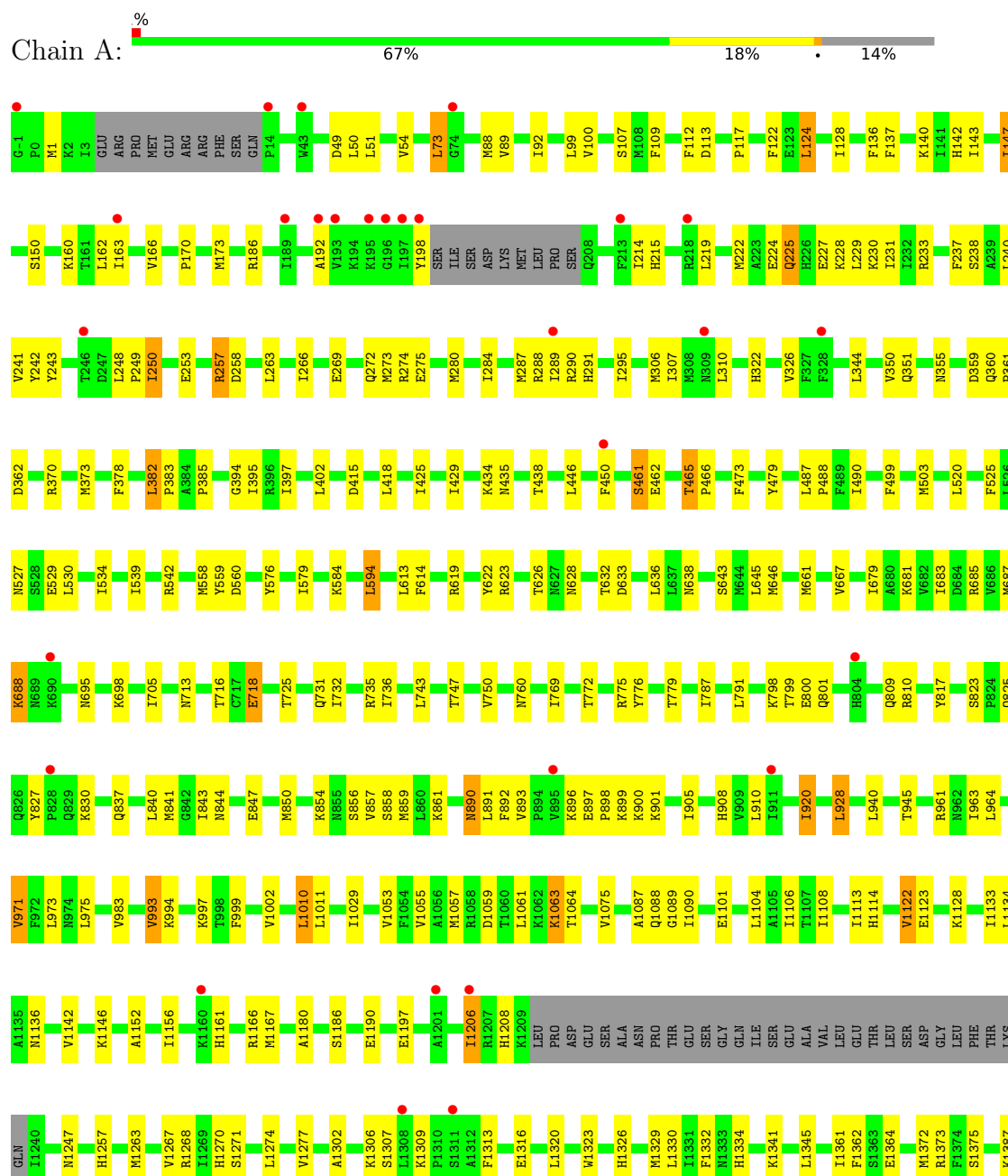
There are 6 discrepancies between the modelled and reference sequences:

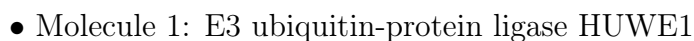
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A177ELV2
A	0	PRO	-	expression tag	UNP A0A177ELV2
A	2457	ALA	CYS	engineered mutation	UNP A0A177ELV2
B	-1	GLY	-	expression tag	UNP A0A177ELV2
B	0	PRO	-	expression tag	UNP A0A177ELV2
B	2457	ALA	CYS	engineered mutation	UNP A0A177ELV2

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: E3 ubiquitin-protein ligase HUWE1





P249	P166	G-1
L250	P167	P0
E253	P170	M1
R257	M173	I3
D258	M174	GLU
I266	M175	ARG
E269	M176	PRO
Q272	M177	MET
M273	C184	GLU
R274	K185	ARG
E275	L186	ARG
M280	L187	PHE
M287	L188	GLN
R288	L189	P14
I289	K190	D49
R290	K191	L50
H291	L192	L51
I295	L193	G74
H303	K194	P80
M306	K195	M81
I307	L196	K82
L310	L197	E83
K313	L198	S84
H322	I1E	D85
V326	SER	M88
S337	ASP	V89
V341	LYS	I92
L344	MET	L99
V350	LEU	V100
Q351	P206	F112
N355	E209	D113
D359	F213	V134
P361	L214	S135
D362	H215	F136
R370	L219	F137
M373	E227	K140
	K230	I141
	L231	H142
	L232	I143
	R233	Q144
	F237	R145
	S238	S146
	A239	I147
	L240	E157
	V241	L162
	Y242	I163
	N244	
	L245	
	L246	
	L247	
	L248	
	L249	
	L250	



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.52Å 96.22Å 199.66Å 92.22° 100.45° 95.33°	Depositor
Resolution (Å)	196.03 – 3.04 196.03 – 3.04	Depositor EDS
% Data completeness (in resolution range)	56.3 (196.03-3.04) 56.3 (196.03-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.202 , 0.233 0.218 , 0.244	Depositor DCC
R_{free} test set	3733 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 83.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34901	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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

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	0.64	0/17792	1.11	27/24002 (0.1%)
1	B	0.64	0/17785	1.11	26/23989 (0.1%)
All	All	0.64	0/35577	1.11	53/47991 (0.1%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	ASP	CA-CB-CG	8.43	121.03	112.60
1	A	378	PHE	CA-CB-CG	8.09	121.89	113.80
1	B	378	PHE	CA-CB-CG	7.88	121.68	113.80
1	B	290	ARG	CA-C-N	7.40	130.51	120.38
1	B	290	ARG	C-N-CA	7.40	130.51	120.38
1	A	290	ARG	CA-C-N	7.31	130.40	120.38
1	A	290	ARG	C-N-CA	7.31	130.40	120.38
1	A	2071	ILE	N-CA-C	7.08	114.00	107.56
1	B	2071	ILE	N-CA-C	6.96	113.90	107.56
1	A	1063	LYS	CA-C-N	6.45	133.85	121.54
1	A	1063	LYS	C-N-CA	6.45	133.85	121.54
1	A	1794	ASN	CA-CB-CG	6.42	119.02	112.60
1	B	1063	LYS	CA-C-N	6.40	133.76	121.54
1	B	1063	LYS	C-N-CA	6.40	133.76	121.54
1	A	2114	ASP	CA-CB-CG	6.39	119.00	112.60
1	B	461	SER	CA-C-N	6.28	129.54	120.38
1	B	461	SER	C-N-CA	6.28	129.54	120.38
1	A	1167	MET	CA-C-N	6.24	128.96	120.54
1	A	1167	MET	C-N-CA	6.24	128.96	120.54
1	A	614	PHE	CA-CB-CG	-6.20	107.60	113.80
1	B	614	PHE	CA-CB-CG	-6.20	107.60	113.80
1	B	2062	ASN	CA-C-N	6.15	133.29	121.54
1	B	2062	ASN	C-N-CA	6.15	133.29	121.54
1	B	2114	ASP	CA-CB-CG	6.13	118.73	112.60
1	B	1403	ASP	CA-CB-CG	6.11	118.70	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	SER	CA-C-N	6.08	129.25	120.38
1	A	461	SER	C-N-CA	6.08	129.25	120.38
1	B	2105	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	1206	ILE	CA-C-N	5.84	129.58	120.82
1	A	1206	ILE	C-N-CA	5.84	129.58	120.82
1	A	1061	LEU	CA-C-N	5.83	133.59	123.91
1	A	1061	LEU	C-N-CA	5.83	133.59	123.91
1	A	1029	ILE	N-CA-CB	5.79	114.40	110.52
1	B	1880	SER	CA-C-N	5.71	128.40	120.29
1	B	1880	SER	C-N-CA	5.71	128.40	120.29
1	A	1180	ALA	CA-C-N	5.69	127.83	120.44
1	A	1180	ALA	C-N-CA	5.69	127.83	120.44
1	A	2052	VAL	N-CA-CB	5.55	117.04	110.55
1	A	1403	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	2194	PHE	CA-C-N	5.43	129.46	120.94
1	A	2194	PHE	C-N-CA	5.43	129.46	120.94
1	B	244	ASN	CA-CB-CG	5.36	117.96	112.60
1	B	2347	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	890	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	2347	PHE	CA-CB-CG	-5.30	108.50	113.80
1	B	2194	PHE	CA-C-N	5.28	129.23	120.94
1	B	2194	PHE	C-N-CA	5.28	129.23	120.94
1	B	1244	SER	N-CA-C	5.27	116.72	110.97
1	B	598	ILE	N-CA-CB	5.23	114.02	110.52
1	B	209	GLU	CA-C-N	5.08	126.96	120.56
1	B	209	GLU	C-N-CA	5.08	126.96	120.56
1	A	1362	PHE	CA-CB-CG	-5.03	108.77	113.80
1	B	890	ASN	CA-CB-CG	5.02	117.62	112.60

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	17453	0	17745	274	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	17448	0	17737	270	0
All	All	34901	0	35482	544	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 8.

All (544) 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:1059:ASP:HA	1:A:1063:LYS:HB3	1.29	1.15
1:B:1059:ASP:HA	1:B:1063:LYS:HB3	1.28	1.15
1:A:2282:ILE:HG12	1:A:2286:LEU:HG	1.33	1.05
1:A:225:GLN:HE21	1:A:228:LYS:NZ	1.55	1.03
1:A:1987:HIS:CE1	1:A:1991:ILE:HD11	1.97	0.99
1:B:1987:HIS:CE1	1:B:1991:ILE:HD11	1.97	0.99
1:A:731:GLN:HE21	1:A:735:ARG:HH21	1.10	0.96
1:B:825:GLN:HE21	1:B:831:ASN:HD21	1.09	0.93
1:B:731:GLN:HE21	1:B:735:ARG:HH21	1.11	0.92
1:B:858:SER:HA	1:B:861:LYS:HD2	1.56	0.88
1:B:1882:ASN:HB3	1:B:1885:LEU:HG	1.56	0.88
1:A:798:LYS:HE2	1:A:810:ARG:HE	1.39	0.87
1:A:1882:ASN:HB3	1:A:1885:LEU:HG	1.58	0.86
1:B:825:GLN:HE21	1:B:831:ASN:ND2	1.73	0.85
1:A:858:SER:HA	1:A:861:LYS:HD2	1.56	0.85
1:A:1987:HIS:ND1	1:A:1991:ILE:HD11	1.92	0.85
1:A:225:GLN:HE21	1:A:228:LYS:HZ3	1.23	0.84
1:A:248:LEU:HG	1:A:249:PRO:HD2	1.59	0.84
1:B:1987:HIS:ND1	1:B:1991:ILE:HD11	1.94	0.83
1:B:248:LEU:HG	1:B:249:PRO:HD2	1.59	0.82
1:A:2192:GLU:O	1:A:2195:ASN:HB2	1.79	0.81
1:A:2091:ASN:HD22	1:A:2117:ASN:HD22	1.27	0.81
1:B:731:GLN:NE2	1:B:735:ARG:HH21	1.78	0.81
1:A:731:GLN:NE2	1:A:735:ARG:HH21	1.79	0.80
1:A:695:ASN:HA	1:A:698:LYS:HD2	1.63	0.79
1:A:731:GLN:HE21	1:A:735:ARG:NH2	1.81	0.79
1:B:731:GLN:HE21	1:B:735:ARG:NH2	1.81	0.79
1:B:215:HIS:NE2	1:B:219:LEU:HD21	1.98	0.78
1:B:725:THR:HG22	1:B:787:ILE:HD11	1.66	0.78
1:A:215:HIS:NE2	1:A:219:LEU:HD21	1.98	0.78
1:B:695:ASN:HA	1:B:698:LYS:HD2	1.64	0.77
1:A:725:THR:HG22	1:A:787:ILE:HD11	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1880:SER:HB3	1:A:1911:CYS:HB2	1.68	0.75
1:B:1880:SER:HB3	1:B:1911:CYS:HB2	1.67	0.74
1:A:687:MET:HE1	1:A:736:ILE:HG12	1.71	0.73
1:A:2133:ARG:HH12	1:A:2236:TYR:HE2	1.37	0.73
1:B:973:LEU:HD21	1:B:1002:VAL:HG12	1.72	0.72
1:A:890:ASN:HB2	1:A:893:VAL:HB	1.70	0.72
1:B:269:GLU:O	1:B:274:ARG:HD2	1.89	0.71
1:A:973:LEU:HD21	1:A:1002:VAL:HG12	1.72	0.71
1:B:890:ASN:HB2	1:B:893:VAL:HB	1.72	0.71
1:B:82:LYS:NZ	1:B:84:SER:HB3	2.06	0.70
1:B:687:MET:HE1	1:B:736:ILE:HG12	1.72	0.70
1:A:225:GLN:NE2	1:A:228:LYS:HZ3	1.89	0.70
1:A:743:LEU:HB3	1:A:750:VAL:HG21	1.74	0.70
1:A:2030:LEU:HG	1:A:2034:LYS:HE3	1.73	0.70
1:A:1257:HIS:ND1	1:A:1268:ARG:NH2	2.40	0.69
1:B:142:HIS:ND1	1:B:287:MET:HE1	2.06	0.69
1:A:142:HIS:ND1	1:A:287:MET:HE1	2.07	0.69
1:B:2030:LEU:HG	1:B:2034:LYS:HE3	1.73	0.69
1:A:825:GLN:HE22	1:A:830:LYS:H	1.41	0.68
1:B:743:LEU:HB3	1:B:750:VAL:HG21	1.75	0.68
1:A:847:GLU:HA	1:A:908:HIS:CE1	2.29	0.67
1:B:175:THR:HG22	1:B:186:ARG:HG2	1.76	0.67
1:A:1982:ASN:HB3	1:A:1985:THR:HB	1.75	0.67
1:B:370:ARG:HE	1:B:373:MET:HE1	1.60	0.67
1:B:1982:ASN:HB3	1:B:1985:THR:HB	1.76	0.66
1:A:370:ARG:HE	1:A:373:MET:HE1	1.60	0.66
1:B:303:HIS:HD1	1:B:2038:TYR:HD2	1.43	0.66
1:A:837:GLN:HG2	1:A:841:MET:HE2	1.77	0.66
1:B:837:GLN:HG2	1:B:841:MET:HE2	1.76	0.66
1:A:275:GLU:CD	1:A:322:HIS:HD2	2.04	0.65
1:B:685:ARG:HA	1:B:688:LYS:HE3	1.78	0.65
1:B:2192:GLU:O	1:B:2195:ASN:HB2	1.95	0.65
1:B:1990:ILE:HD12	1:B:2044:PRO:HB2	1.79	0.65
1:B:996:LYS:NZ	1:B:1024:HIS:HD2	1.95	0.65
1:A:1990:ILE:HD12	1:A:2044:PRO:HB2	1.77	0.65
1:B:2212:HIS:NE2	1:B:2334:VAL:HG11	2.11	0.64
1:A:685:ARG:HA	1:A:688:LYS:HE3	1.78	0.64
1:A:2288:MET:HE3	1:A:2314:VAL:HG21	1.78	0.64
1:B:163:ILE:HD11	1:B:240:LEU:HD12	1.79	0.64
1:A:827:TYR:HD2	1:A:830:LYS:HB2	1.63	0.63
1:B:82:LYS:HZ2	1:B:84:SER:HB3	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1258:ARG:HH22	1:B:1293:PHE:HD1	1.46	0.63
1:B:173:MET:HG3	1:B:188:SER:HA	1.80	0.63
1:B:303:HIS:ND1	1:B:2038:TYR:HD2	1.97	0.63
1:A:128:ILE:HD11	1:A:231:ILE:HG13	1.80	0.62
1:A:2161:VAL:HG11	1:A:2229:ARG:HD3	1.81	0.62
1:A:1257:HIS:CE1	1:A:1268:ARG:HH22	2.17	0.62
1:A:891:LEU:HG	1:A:892:PHE:HD1	1.65	0.62
1:B:844:ASN:HB3	1:B:847:GLU:HB3	1.82	0.62
1:A:163:ILE:HD11	1:A:240:LEU:HD12	1.81	0.61
1:B:429:ILE:HG13	1:B:450:PHE:CZ	2.35	0.61
1:B:1945:CYS:O	1:B:1949:LYS:HG3	2.00	0.61
1:A:920:ILE:HD11	1:A:975:LEU:HD11	1.82	0.61
1:A:2274:LEU:HD22	1:A:2323:VAL:HG22	1.83	0.61
1:B:2161:VAL:HG11	1:B:2229:ARG:HD3	1.81	0.61
1:B:1152:ALA:O	1:B:1156:ILE:HG12	2.01	0.61
1:A:1186:SER:O	1:A:1190:GLU:HG2	2.01	0.61
1:B:1786:VAL:HG12	1:B:1795:LEU:HD22	1.83	0.61
1:A:844:ASN:HB3	1:A:847:GLU:HB3	1.83	0.60
1:A:1152:ALA:O	1:A:1156:ILE:HG12	2.01	0.60
1:A:1403:ASP:HA	1:A:1409:TYR:CE2	2.36	0.60
1:B:2133:ARG:HD3	1:B:2165:LYS:HZ3	1.66	0.60
1:A:222:MET:HE3	1:A:225:GLN:HB2	1.83	0.60
1:A:1101:GLU:HG2	1:A:1146:LYS:HG3	1.83	0.60
1:A:1786:VAL:HG12	1:A:1795:LEU:HD22	1.83	0.60
1:B:227:GLU:OE1	1:B:272:GLN:NE2	2.33	0.60
1:B:1101:GLU:HG2	1:B:1146:LYS:HG3	1.83	0.60
1:A:1789:CYS:O	1:A:1792:ARG:HD3	2.02	0.60
1:A:88:MET:O	1:A:92:ILE:HG12	2.02	0.59
1:B:771:LYS:O	1:B:775:ARG:HG2	2.02	0.59
1:B:858:SER:HA	1:B:861:LYS:CD	2.30	0.59
1:A:429:ILE:HG13	1:A:450:PHE:CZ	2.37	0.59
1:A:856:SER:HA	1:A:859:MET:HE2	1.84	0.59
1:A:231:ILE:HG21	1:A:273:MET:HA	1.84	0.59
1:A:225:GLN:HG3	1:A:228:LYS:HZ3	1.67	0.59
1:B:88:MET:O	1:B:92:ILE:HG12	2.02	0.59
1:B:100:VAL:HG23	1:B:136:PHE:HE2	1.68	0.58
1:A:643:SER:HA	1:A:646:MET:HE2	1.85	0.58
1:A:718:GLU:CD	1:A:718:GLU:H	2.11	0.58
1:B:2274:LEU:HD22	1:B:2323:VAL:HG22	1.84	0.58
1:A:993:VAL:HG22	1:A:999:PHE:HA	1.84	0.58
1:B:275:GLU:CD	1:B:322:HIS:HD2	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:914:GLU:HA	1:B:917:MET:HE2	1.85	0.58
1:A:2223:TYR:O	1:A:2227:ILE:HG12	2.02	0.58
1:B:177:TYR:HB3	1:B:1406:ARG:HD3	1.84	0.58
1:B:2014:MET:HE1	1:B:2074:SER:HA	1.85	0.58
1:A:269:GLU:O	1:A:274:ARG:HD2	2.03	0.58
1:A:858:SER:HA	1:A:861:LYS:CD	2.30	0.58
1:B:2252:ARG:HG2	1:B:2339:LEU:HG	1.86	0.57
1:A:288:ARG:HA	1:A:291:HIS:HD2	1.70	0.57
1:B:633:ASP:HB3	1:B:636:LEU:HB2	1.87	0.57
1:A:225:GLN:CG	1:A:228:LYS:HZ3	2.18	0.57
1:B:584:LYS:NZ	1:B:633:ASP:HB2	2.19	0.57
1:B:2221:LEU:HD21	1:B:2337:ARG:HB3	1.87	0.57
1:B:394:GLY:HA2	1:B:397:ILE:HD12	1.87	0.57
1:B:2168:ILE:HG21	1:B:2185:TRP:HB2	1.86	0.57
1:A:633:ASP:HB3	1:A:636:LEU:HB2	1.87	0.57
1:A:2221:LEU:HD21	1:A:2337:ARG:HB3	1.86	0.57
1:A:225:GLN:HE21	1:A:228:LYS:HZ1	1.50	0.56
1:A:584:LYS:NZ	1:A:633:ASP:HB2	2.20	0.56
1:A:1395:MET:HE2	1:A:1420:MET:HB3	1.87	0.56
1:A:1332:PHE:HA	1:A:1341:LYS:HE2	1.86	0.56
1:A:2054:THR:HG23	1:A:2107:GLY:HA3	1.87	0.56
1:B:266:ILE:HA	1:B:274:ARG:HB2	1.86	0.56
1:B:718:GLU:H	1:B:718:GLU:CD	2.12	0.56
1:A:394:GLY:HA2	1:A:397:ILE:HD12	1.88	0.56
1:A:2373:ILE:HD11	1:A:2427:PHE:HZ	1.70	0.56
1:A:1997:LEU:HD22	1:A:2052:VAL:HG13	1.86	0.56
1:A:1:MET:HE1	1:A:50:LEU:HD22	1.88	0.56
1:A:2168:ILE:HG21	1:A:2185:TRP:HB2	1.86	0.56
1:A:892:PHE:HD2	1:A:961:ARG:HB3	1.70	0.56
1:B:1768:ARG:HH22	1:B:1800:HIS:CD2	2.24	0.56
1:A:898:PRO:HA	1:A:900:LYS:NZ	2.21	0.56
1:B:996:LYS:HZ1	1:B:1024:HIS:HD2	1.51	0.56
1:B:2151:HIS:CE1	1:B:2155:ARG:HH21	2.24	0.56
1:B:2223:TYR:O	1:B:2227:ILE:HG12	2.05	0.56
1:A:1971:LEU:HD13	1:A:2019:MET:HG3	1.88	0.56
1:A:827:TYR:HB3	1:A:830:LYS:HD3	1.88	0.55
1:B:1395:MET:HE2	1:B:1420:MET:HB3	1.89	0.55
1:A:798:LYS:HE2	1:A:810:ARG:NE	2.18	0.55
1:A:1768:ARG:HH22	1:A:1800:HIS:CD2	2.24	0.55
1:B:1178:ARG:NH1	1:B:1554:ASN:ND2	2.54	0.55
1:B:1868:LEU:O	1:B:1871:LYS:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1932:LEU:HD12	1:B:1962:TYR:HE2	1.71	0.55
1:A:2187:SER:O	1:A:2191:LYS:HG3	2.05	0.55
1:A:503:MET:HE3	1:A:542:ARG:HG3	1.87	0.55
1:A:1868:LEU:O	1:A:1871:LYS:O	2.24	0.55
1:B:1971:LEU:HD13	1:B:2019:MET:HG3	1.89	0.55
1:A:1895:LYS:NZ	1:A:1896:ARG:NH2	2.53	0.55
1:A:2151:HIS:CE1	1:A:2155:ARG:HH21	2.25	0.55
1:A:2291:SER:HB3	1:A:2310:ARG:HA	1.89	0.55
1:B:1326:HIS:NE2	1:B:1330:LEU:HD21	2.22	0.55
1:B:2291:SER:HB3	1:B:2310:ARG:HA	1.89	0.55
1:A:898:PRO:HA	1:A:900:LYS:HZ3	1.72	0.55
1:A:288:ARG:HA	1:A:291:HIS:CD2	2.42	0.54
1:B:920:ILE:HG21	1:B:928:LEU:HD12	1.89	0.54
1:B:2195:ASN:HB3	1:B:2198:TYR:HB2	1.90	0.54
1:B:1326:HIS:CD2	1:B:1330:LEU:HD23	2.42	0.54
1:A:1895:LYS:HZ1	1:A:1896:ARG:NH2	2.06	0.54
1:A:2195:ASN:HB3	1:A:2198:TYR:HB2	1.90	0.54
1:B:1925:VAL:HG12	1:B:1958:MET:HE2	1.89	0.54
1:B:415:ASP:HB3	1:B:418:LEU:HB3	1.90	0.54
1:B:2187:SER:O	1:B:2191:LYS:HG2	2.08	0.54
1:A:382:LEU:O	1:A:385:PRO:HD2	2.08	0.53
1:B:382:LEU:O	1:B:385:PRO:HD2	2.08	0.53
1:B:556:ILE:O	1:B:559:TYR:O	2.26	0.53
1:A:683:ILE:HG12	1:A:687:MET:HE3	1.91	0.53
1:B:2209:GLN:HB3	1:B:2246:THR:CG2	2.38	0.53
1:A:638:ASN:HB2	1:A:667:VAL:HG11	1.90	0.53
1:A:1161:HIS:CD2	1:A:1208:HIS:NE2	2.77	0.53
1:B:731:GLN:NE2	1:B:735:ARG:NH2	2.49	0.53
1:B:1161:HIS:NE2	1:B:1208:HIS:CE1	2.76	0.53
1:A:122:PHE:HE1	1:A:214:ILE:HG23	1.72	0.53
1:B:1002:VAL:HG23	1:B:1011:LEU:HD11	1.90	0.53
1:A:1330:LEU:HD22	1:A:1334:HIS:CD2	2.44	0.53
1:B:503:MET:HE3	1:B:542:ARG:HG3	1.90	0.53
1:B:191:LYS:HG2	1:B:193:VAL:HG22	1.90	0.53
1:B:718:GLU:HB3	1:B:776:TYR:OH	2.09	0.53
1:A:1925:VAL:HG12	1:A:1958:MET:HE2	1.91	0.53
1:A:2209:GLN:HB3	1:A:2246:THR:CG2	2.39	0.53
1:B:2005:ILE:HG13	1:B:2009:TYR:HB2	1.91	0.52
1:A:731:GLN:NE2	1:A:735:ARG:NH2	2.50	0.52
1:B:683:ILE:HG12	1:B:687:MET:HE3	1.90	0.52
1:B:1345:LEU:HD13	1:B:1389:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:VAL:HG12	1:A:983:VAL:O	2.10	0.52
1:A:1197:GLU:HA	1:A:1208:HIS:CD2	2.44	0.52
1:B:435:ASN:HD22	1:B:438:THR:H	1.58	0.52
1:A:415:ASP:HB3	1:A:418:LEU:HB3	1.90	0.52
1:B:242:TYR:HD1	1:B:287:MET:HE3	1.75	0.52
1:B:303:HIS:ND1	1:B:2038:TYR:CD2	2.72	0.52
1:A:1891:GLN:HG2	1:A:1927:LYS:NZ	2.25	0.52
1:B:1270:HIS:NE2	1:B:1274:LEU:HD11	2.25	0.51
1:A:840:LEU:HD23	1:A:843:ILE:HD11	1.93	0.51
1:B:2054:THR:HG23	1:B:2107:GLY:HA3	1.91	0.51
1:A:160:LYS:HA	1:A:163:ILE:HG12	1.92	0.51
1:A:1307:SER:HB2	1:A:1364:GLU:OE2	2.10	0.51
1:A:1345:LEU:HD13	1:A:1389:MET:HG3	1.92	0.51
1:A:2133:ARG:NH1	1:A:2236:TYR:HE2	2.08	0.51
1:B:1891:GLN:HG2	1:B:1927:LYS:NZ	2.26	0.51
1:B:1953:ARG:HD3	1:B:2061:ARG:HD2	1.92	0.51
1:A:718:GLU:HB3	1:A:776:TYR:OH	2.10	0.51
1:A:192:ALA:HA	1:A:198:TYR:HD1	1.76	0.51
1:A:284:ILE:HG23	1:A:289:ILE:HG23	1.92	0.51
1:A:1002:VAL:HG23	1:A:1011:LEU:HD11	1.92	0.51
1:B:983:VAL:HG12	1:B:983:VAL:O	2.11	0.51
1:B:1422:TYR:CE2	1:B:1426:ILE:HD11	2.45	0.51
1:B:2260:LEU:HG	1:B:2271:HIS:CE1	2.46	0.51
1:B:638:ASN:HB2	1:B:667:VAL:HG11	1.92	0.51
1:B:1175:SER:HA	1:B:1178:ARG:HG3	1.91	0.51
1:B:1949:LYS:HG2	1:B:2002:ILE:HG21	1.93	0.51
1:B:2135:THR:HA	1:B:2165:LYS:HB2	1.93	0.51
1:B:973:LEU:HB3	1:B:1005:LYS:HD2	1.91	0.51
1:A:823:SER:OG	1:A:830:LYS:O	2.29	0.51
1:B:766:THR:HA	1:B:769:ILE:HG12	1.93	0.51
1:B:913:VAL:O	1:B:917:MET:HG3	2.10	0.51
1:B:1345:LEU:HB3	1:B:1389:MET:HE2	1.93	0.51
1:A:1270:HIS:NE2	1:A:1274:LEU:HD11	2.26	0.50
1:A:2252:ARG:HG2	1:A:2339:LEU:HG	1.93	0.50
1:B:499:PHE:O	1:B:503:MET:HG2	2.11	0.50
1:B:177:TYR:HD1	1:B:184:CYS:HB3	1.76	0.50
1:B:2209:GLN:HB3	1:B:2246:THR:HG21	1.93	0.50
1:A:250:ILE:HD13	1:A:289:ILE:HD11	1.92	0.50
1:B:215:HIS:CD2	1:B:219:LEU:HD21	2.47	0.50
1:A:2135:THR:HA	1:A:2165:LYS:HB2	1.94	0.50
1:A:1142:VAL:O	1:A:1247:ASN:OD1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1257:HIS:CE1	1:A:1268:ARG:NH2	2.78	0.50
1:A:435:ASN:HD22	1:A:438:THR:H	1.58	0.50
1:A:791:LEU:HB3	1:A:817:TYR:CE2	2.47	0.50
1:A:402:LEU:HB2	1:A:425:ILE:HG21	1.93	0.50
1:A:2209:GLN:HB3	1:A:2246:THR:HG21	1.94	0.50
1:B:2335:ILE:HG23	1:B:2339:LEU:HD23	1.94	0.50
1:B:1307:SER:HB2	1:B:1364:GLU:OE2	2.11	0.49
1:A:850:MET:HE3	1:A:854:LYS:HE2	1.94	0.49
1:B:713:ASN:ND2	1:B:716:THR:OG1	2.46	0.49
1:B:1002:VAL:CG2	1:B:1011:LEU:HD11	2.43	0.49
1:A:1088:GLN:HE21	1:A:1114:HIS:HE1	1.60	0.49
1:A:1323:TRP:NE1	1:A:1537:LEU:CD1	2.75	0.49
1:A:2378:TRP:O	1:A:2382:THR:OG1	2.29	0.49
1:B:2247:ARG:NH1	1:B:2250:TYR:CD2	2.80	0.49
1:A:2335:ILE:HG23	1:A:2339:LEU:HD23	1.94	0.49
1:B:1277:VAL:HG22	1:B:1334:HIS:CE1	2.46	0.49
1:A:791:LEU:HB3	1:A:817:TYR:HE2	1.77	0.49
1:B:192:ALA:HA	1:B:198:TYR:HD2	1.77	0.49
1:B:465:THR:HG22	1:B:466:PRO:HD2	1.94	0.49
1:B:1104:LEU:HD11	1:B:1106:ILE:HD12	1.94	0.49
1:B:1332:PHE:HA	1:B:1341:LYS:HE2	1.95	0.49
1:B:142:HIS:CE1	1:B:287:MET:HE1	2.48	0.49
1:A:1949:LYS:HG2	1:A:2002:ILE:HG21	1.94	0.49
1:B:167:LYS:HD2	1:B:170:PRO:HB3	1.94	0.49
1:B:2049:PHE:O	1:B:2053:HIS:HD2	1.96	0.49
1:A:124:LEU:HD22	1:A:225:GLN:HB3	1.95	0.49
1:A:359:ASP:O	1:A:361:PRO:HD3	2.12	0.49
1:B:928:LEU:HD13	1:B:971:VAL:HG11	1.94	0.49
1:A:107:SER:HB3	1:A:147:ILE:HG22	1.93	0.49
1:A:1309:LYS:HZ3	1:A:1313:PHE:HE1	1.60	0.49
1:B:359:ASP:O	1:B:361:PRO:HD3	2.13	0.49
1:B:1089:GLY:HA3	1:B:1134:LEU:HD21	1.95	0.49
1:A:760:ASN:HD21	1:A:809:GLN:HE21	1.60	0.48
1:A:1550:MET:HE3	1:A:1554:ASN:HB3	1.95	0.48
1:B:1396:ILE:HG22	1:B:1400:MET:HE2	1.94	0.48
1:A:465:THR:HG22	1:A:466:PRO:HD2	1.96	0.48
1:A:2247:ARG:HA	1:A:2247:ARG:HD3	1.61	0.48
1:B:402:LEU:HB2	1:B:425:ILE:HG21	1.94	0.48
1:A:525:PHE:HB3	1:A:576:TYR:CE1	2.48	0.48
1:B:1133:ILE:HD13	1:B:1548:LYS:HD2	1.95	0.48
1:B:1323:TRP:NE1	1:B:1537:LEU:CD1	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:O	1:A:233:ARG:HG2	2.13	0.48
1:A:1323:TRP:NE1	1:A:1537:LEU:HD12	2.29	0.48
1:A:382:LEU:HB3	1:A:385:PRO:CD	2.44	0.48
1:A:584:LYS:HZ2	1:A:633:ASP:HB2	1.77	0.48
1:A:1345:LEU:HB3	1:A:1389:MET:HE2	1.95	0.48
1:B:791:LEU:HB3	1:B:817:TYR:CE2	2.48	0.48
1:A:215:HIS:CD2	1:A:219:LEU:HD21	2.49	0.48
1:A:242:TYR:HD1	1:A:287:MET:HE3	1.79	0.48
1:A:910:LEU:HD23	1:A:964:LEU:HD13	1.96	0.48
1:A:1396:ILE:HG22	1:A:1400:MET:HE2	1.95	0.48
1:B:791:LEU:HB3	1:B:817:TYR:HE2	1.78	0.48
1:B:1816:LEU:HB3	1:B:1865:LEU:HG	1.96	0.48
1:A:1104:LEU:HD11	1:A:1106:ILE:HD12	1.95	0.48
1:B:382:LEU:HB3	1:B:385:PRO:CD	2.43	0.48
1:B:622:TYR:H	1:B:632:THR:HG21	1.79	0.48
1:B:1323:TRP:NE1	1:B:1537:LEU:HD12	2.29	0.48
1:B:1429:VAL:HG21	1:B:1437:GLU:HG3	1.94	0.48
1:A:225:GLN:NE2	1:A:228:LYS:NZ	2.39	0.48
1:A:1133:ILE:HD13	1:A:1548:LYS:HD2	1.96	0.48
1:B:503:MET:HE2	1:B:539:ILE:HG23	1.96	0.48
1:A:928:LEU:HD13	1:A:971:VAL:HG11	1.96	0.47
1:A:1816:LEU:HB3	1:A:1865:LEU:HG	1.96	0.47
1:B:661:MET:HE1	1:B:705:ILE:HG22	1.96	0.47
1:A:266:ILE:HA	1:A:274:ARG:HB2	1.96	0.47
1:A:1010:LEU:HD23	1:A:1011:LEU:HD12	1.96	0.47
1:A:1330:LEU:HD23	1:A:1372:MET:HE1	1.96	0.47
1:A:1277:VAL:HG22	1:A:1334:HIS:CE1	2.49	0.47
1:A:623:ARG:H	1:A:628:ASN:ND2	2.13	0.47
1:A:142:HIS:CE1	1:A:287:MET:HE1	2.49	0.47
1:A:622:TYR:H	1:A:632:THR:HG21	1.79	0.47
1:B:230:LYS:O	1:B:233:ARG:HG2	2.14	0.47
1:B:760:ASN:HD21	1:B:809:GLN:HE21	1.61	0.47
1:B:1326:HIS:CD2	1:B:1330:LEU:CD2	2.97	0.47
1:A:1326:HIS:ND1	1:A:1329:MET:CE	2.78	0.47
1:A:2272:ARG:HA	1:A:2275:VAL:HG22	1.97	0.47
1:B:903:CYS:SG	1:B:960:ARG:NH2	2.87	0.47
1:B:1016:ILE:HG12	1:B:1054:PHE:CE1	2.50	0.47
1:B:615:ARG:NH2	1:B:618:HIS:ND1	2.60	0.47
1:B:910:LEU:HD23	1:B:964:LEU:HD13	1.97	0.47
1:B:1905:LEU:HA	1:B:1908:VAL:HB	1.97	0.47
1:A:2361:LYS:HD3	1:A:2414:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2305:LEU:HD13	1:B:2325:LEU:HB3	1.96	0.47
1:A:382:LEU:HB3	1:A:385:PRO:HD3	1.97	0.47
1:B:623:ARG:H	1:B:628:ASN:ND2	2.12	0.47
1:B:1326:HIS:ND1	1:B:1329:MET:CE	2.77	0.47
1:B:2059:ILE:HG23	1:B:2068:PHE:HB2	1.97	0.47
1:A:499:PHE:O	1:A:503:MET:HG2	2.15	0.46
1:B:1524:SER:HA	1:B:1527:GLN:HB3	1.97	0.46
1:B:238:SER:HB3	1:B:280:MET:HA	1.97	0.46
1:B:558:MET:SD	1:B:559:TYR:CE2	3.08	0.46
1:A:227:GLU:HB2	1:A:273:MET:SD	2.55	0.46
1:A:1413:MET:HE2	1:A:1795:LEU:HD11	1.97	0.46
1:A:2047:LYS:O	1:A:2051:ILE:HG13	2.14	0.46
1:B:382:LEU:HB3	1:B:385:PRO:HD3	1.97	0.46
1:B:774:TYR:HD1	1:B:775:ARG:NH2	2.12	0.46
1:B:899:LYS:HA	1:B:900:LYS:HZ2	1.79	0.46
1:A:238:SER:HB3	1:A:280:MET:HA	1.96	0.46
1:A:487:LEU:N	1:A:488:PRO:HD2	2.31	0.46
1:A:840:LEU:HA	1:A:843:ILE:HG12	1.97	0.46
1:B:142:HIS:CE1	1:B:287:MET:CE	2.98	0.46
1:A:732:ILE:O	1:A:736:ILE:HG13	2.16	0.46
1:A:897:GLU:HB3	1:A:898:PRO:HD3	1.97	0.46
1:B:1161:HIS:CD2	1:B:1208:HIS:CE1	3.04	0.46
1:A:1002:VAL:CG2	1:A:1011:LEU:HD11	2.45	0.46
1:A:1323:TRP:HE1	1:A:1537:LEU:HD12	1.81	0.46
1:A:1905:LEU:HA	1:A:1908:VAL:HB	1.98	0.46
1:A:2084:GLU:HG2	1:A:2087:LYS:HD3	1.97	0.46
1:B:2101:LEU:HD21	1:B:2113:LEU:HD11	1.98	0.46
1:A:1087:ALA:HA	1:A:1090:ILE:HD12	1.98	0.46
1:B:645:LEU:HD13	1:B:705:ILE:HG21	1.97	0.46
1:B:732:ILE:O	1:B:736:ILE:HG13	2.16	0.46
1:B:1330:LEU:CD1	1:B:1334:HIS:CD2	2.99	0.46
1:B:1550:MET:HE3	1:B:1554:ASN:HB3	1.97	0.46
1:A:1306:LYS:HZ3	1:A:1361:ILE:HD11	1.79	0.46
1:B:2463:LEU:HD21	1:B:2472:LEU:HD11	1.97	0.46
1:A:73:LEU:HD12	1:A:117:PRO:HG3	1.97	0.45
1:A:1330:LEU:CD2	1:A:1334:HIS:CD2	2.99	0.45
1:A:351:GLN:O	1:A:355:ASN:OD1	2.33	0.45
1:A:1975:LEU:HD22	1:A:1978:LYS:HD3	1.97	0.45
1:B:847:GLU:HA	1:B:908:HIS:CE1	2.51	0.45
1:B:1882:ASN:CB	1:B:1885:LEU:HG	2.39	0.45
1:A:100:VAL:HG23	1:A:136:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2433:GLN:H	1:A:2433:GLN:HG3	1.60	0.45
1:B:257:ARG:HG3	1:B:258:ASP:N	2.32	0.45
1:B:351:GLN:O	1:B:355:ASN:OD1	2.33	0.45
1:B:1123:GLU:HA	1:B:1263:MET:HG2	1.99	0.45
1:A:142:HIS:CE1	1:A:287:MET:CE	2.99	0.45
1:A:291:HIS:CE1	1:A:295:ILE:HD11	2.51	0.45
1:A:2305:LEU:HD13	1:A:2325:LEU:HB3	1.97	0.45
1:B:1161:HIS:CE1	1:B:1208:HIS:CE1	3.05	0.45
1:B:1323:TRP:HE1	1:B:1537:LEU:HD12	1.82	0.45
1:B:1975:LEU:HD22	1:B:1978:LYS:HD3	1.97	0.45
1:A:503:MET:HE2	1:A:539:ILE:HG23	1.98	0.45
1:A:645:LEU:HD13	1:A:705:ILE:HG21	1.97	0.45
1:B:996:LYS:NZ	1:B:1024:HIS:CD2	2.80	0.45
1:B:1198:CYS:SG	1:B:1208:HIS:CD2	3.10	0.45
1:B:1413:MET:HE2	1:B:1795:LEU:HD11	1.98	0.45
1:A:1326:HIS:ND1	1:A:1329:MET:HE2	2.32	0.45
1:B:969:ILE:HD11	1:B:992:LEU:HD13	1.99	0.45
1:B:1768:ARG:O	1:B:1809:ARG:NH2	2.50	0.45
1:A:713:ASN:ND2	1:A:716:THR:OG1	2.50	0.45
1:A:844:ASN:HD21	1:A:901:LYS:HZ2	1.65	0.45
1:A:772:THR:HG22	1:A:775:ARG:HH11	1.82	0.44
1:B:1166:ARG:H	1:B:1166:ARG:HG3	1.60	0.44
1:A:1549:GLU:O	1:A:1552:ILE:HG12	2.18	0.44
1:B:291:HIS:CE1	1:B:295:ILE:HD11	2.52	0.44
1:A:2448:SER:HB2	1:A:2471:GLN:OE1	2.17	0.44
1:B:1426:ILE:HG23	1:B:1434:ALA:HB1	1.98	0.44
1:B:2334:VAL:O	1:B:2335:ILE:HD12	2.16	0.44
1:A:257:ARG:HG3	1:A:258:ASP:N	2.32	0.44
1:B:487:LEU:N	1:B:488:PRO:HD2	2.32	0.44
1:B:2056:GLN:HB2	1:B:2058:TYR:CE1	2.53	0.44
1:A:801:GLN:NE2	1:A:810:ARG:NH2	2.66	0.44
1:A:1945:CYS:O	1:A:1949:LYS:HG3	2.18	0.44
1:B:288:ARG:HA	1:B:291:HIS:CD2	2.52	0.44
1:B:910:LEU:HD13	1:B:963:ILE:HD11	1.98	0.44
1:B:1326:HIS:ND1	1:B:1329:MET:HE2	2.33	0.44
1:A:109:PHE:O	1:A:150:SER:OG	2.36	0.44
1:A:2101:LEU:HD21	1:A:2113:LEU:HD11	2.00	0.44
1:A:350:VAL:HG21	1:A:385:PRO:HB3	2.00	0.44
1:B:584:LYS:HZ2	1:B:633:ASP:HB2	1.82	0.44
1:B:2448:SER:HB2	1:B:2471:GLN:OE1	2.17	0.44
1:A:173:MET:HB3	1:A:186:ARG:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2258:VAL:HG21	1:B:2331:LEU:HD11	1.99	0.44
1:B:1549:GLU:O	1:B:1552:ILE:HG12	2.18	0.44
1:A:910:LEU:HD13	1:A:963:ILE:HD11	1.99	0.43
1:A:1053:VAL:HG22	1:A:1057:MET:HE3	1.99	0.43
1:A:827:TYR:CD2	1:A:830:LYS:HB2	2.49	0.43
1:A:1895:LYS:HZ2	1:A:1896:ARG:CZ	2.31	0.43
1:B:2052:VAL:HG23	1:B:2053:HIS:CD2	2.53	0.43
1:B:2212:HIS:NE2	1:B:2334:VAL:CG1	2.78	0.43
1:B:2332:VAL:O	1:B:2336:GLU:HB2	2.18	0.43
1:B:2396:TRP:CD1	1:B:2469:TYR:HB2	2.53	0.43
1:A:2025:TYR:CZ	1:A:2045:LEU:HD13	2.54	0.43
1:B:825:GLN:NE2	1:B:831:ASN:ND2	2.53	0.43
1:A:1422:TYR:O	1:A:1426:ILE:HG12	2.18	0.43
1:B:350:VAL:HG21	1:B:385:PRO:HB3	2.00	0.43
1:B:1929:ILE:HG13	1:B:1962:TYR:CD2	2.53	0.43
1:A:225:GLN:HG3	1:A:228:LYS:NZ	2.33	0.43
1:B:162:LEU:HD23	1:B:215:HIS:CE1	2.54	0.43
1:B:1053:VAL:HG22	1:B:1057:MET:HE3	1.99	0.43
1:B:1309:LYS:NZ	1:B:1313:PHE:HE1	2.16	0.43
1:A:558:MET:SD	1:A:559:TYR:CE1	3.12	0.43
1:A:891:LEU:HG	1:A:892:PHE:CD1	2.49	0.43
1:A:2116:ASP:O	1:A:2120:ILE:HG13	2.18	0.43
1:A:162:LEU:HD23	1:A:215:HIS:CE1	2.54	0.43
1:A:1403:ASP:HA	1:A:1409:TYR:HE2	1.83	0.43
1:A:2332:VAL:O	1:A:2336:GLU:HB2	2.19	0.43
1:B:157:GLU:H	1:B:157:GLU:CD	2.27	0.43
1:B:2025:TYR:CZ	1:B:2045:LEU:HD13	2.54	0.43
1:B:2116:ASP:O	1:B:2120:ILE:HG13	2.18	0.43
1:A:215:HIS:O	1:A:219:LEU:HG	2.19	0.43
1:A:1122:VAL:HG11	1:A:1267:VAL:HG21	2.00	0.43
1:A:1309:LYS:NZ	1:A:1313:PHE:HE1	2.17	0.43
1:B:2446:GLY:HA3	1:B:2450:ARG:HD2	2.01	0.43
1:A:1123:GLU:HA	1:A:1263:MET:HG2	2.00	0.43
1:B:215:HIS:O	1:B:219:LEU:HG	2.19	0.43
1:B:1085:VAL:HA	1:B:1088:GLN:HE21	1.84	0.43
1:A:140:LYS:HD3	1:A:143:ILE:HD12	2.01	0.42
1:A:1999:LEU:HD23	1:A:2002:ILE:HD12	2.00	0.42
1:A:2396:TRP:CD1	1:A:2469:TYR:HB2	2.54	0.42
1:B:188:SER:O	1:B:199:SER:O	2.37	0.42
1:B:382:LEU:HG	1:B:383:PRO:HD2	2.01	0.42
1:B:2047:LYS:O	1:B:2051:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LEU:HG	1:A:383:PRO:HD2	2.01	0.42
1:A:661:MET:HE1	1:A:705:ILE:HG22	2.00	0.42
1:A:1891:GLN:CG	1:A:1927:LYS:NZ	2.82	0.42
1:B:307:ILE:HD13	1:B:344:LEU:HD21	2.01	0.42
1:A:49:ASP:HB3	1:A:51:LEU:HD12	2.01	0.42
1:A:892:PHE:CD2	1:A:961:ARG:HB3	2.52	0.42
1:A:1330:LEU:HD23	1:A:1330:LEU:HA	1.96	0.42
1:B:1891:GLN:CG	1:B:1927:LYS:NZ	2.83	0.42
1:A:248:LEU:HG	1:A:249:PRO:CD	2.40	0.42
1:A:527:ASN:HB3	1:A:530:LEU:HG	2.02	0.42
1:A:890:ASN:HB2	1:A:893:VAL:CB	2.46	0.42
1:A:896:LYS:HA	1:A:899:LYS:HE3	2.00	0.42
1:B:556:ILE:HA	1:B:561:ILE:HB	2.01	0.42
1:B:841:MET:HG2	1:B:905:ILE:HD11	2.00	0.42
1:B:2286:LEU:HG	1:B:2288:MET:HB2	2.00	0.42
1:A:360:GLN:HE21	1:A:362:ASP:HB2	1.85	0.42
1:B:1429:VAL:HG12	1:B:1431:GLU:HG2	2.00	0.42
1:B:1118:ILE:HG21	1:B:1135:ALA:HB2	2.01	0.42
1:B:1567:GLU:HA	1:B:1570:ILE:HD12	2.01	0.42
1:B:2030:LEU:CG	1:B:2034:LYS:HE3	2.47	0.42
1:A:1302:ALA:HA	1:A:1361:ILE:HG21	2.01	0.42
1:A:2258:VAL:HG21	1:A:2331:LEU:HD11	2.01	0.42
1:B:237:PHE:O	1:B:241:VAL:HG23	2.20	0.42
1:B:288:ARG:HH11	1:B:337:SER:HB2	1.84	0.42
1:B:1330:LEU:CD1	1:B:1334:HIS:NE2	2.83	0.42
1:B:519:ASN:O	1:B:522:GLU:HG2	2.20	0.42
1:B:2372:GLU:HA	1:B:2406:MET:CG	2.50	0.42
1:A:1136:ASN:HD21	1:A:1271:SER:HA	1.85	0.41
1:B:140:LYS:HD3	1:B:143:ILE:HD12	2.02	0.41
1:B:360:GLN:HE21	1:B:362:ASP:HB2	1.85	0.41
1:B:1122:VAL:HG11	1:B:1267:VAL:HG21	2.02	0.41
1:B:2282:ILE:HD13	1:B:2282:ILE:HA	1.96	0.41
1:B:2397:TYR:HA	1:B:2472:LEU:HD21	2.02	0.41
1:A:307:ILE:HD13	1:A:344:LEU:HD21	2.01	0.41
1:A:479:TYR:CD2	1:A:490:ILE:HD11	2.54	0.41
1:A:1059:ASP:HA	1:A:1063:LYS:CB	2.21	0.41
1:B:1059:ASP:HA	1:B:1063:LYS:CB	2.21	0.41
1:B:1136:ASN:HD21	1:B:1271:SER:HA	1.85	0.41
1:A:128:ILE:CD1	1:A:231:ILE:HG13	2.47	0.41
1:A:844:ASN:HD21	1:A:901:LYS:NZ	2.18	0.41
1:A:1330:LEU:CD2	1:A:1334:HIS:NE2	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2061:ARG:HG3	1:A:2067:GLU:HG2	2.02	0.41
1:B:49:ASP:HB3	1:B:51:LEU:HD12	2.02	0.41
1:B:1999:LEU:HD23	1:B:2002:ILE:HD12	2.01	0.41
1:B:2455:HIS:HB2	1:B:2460:GLN:HB3	2.01	0.41
1:A:1770:ALA:O	1:A:1805:ASN:HB3	2.20	0.41
1:B:579:ILE:H	1:B:579:ILE:HG13	1.75	0.41
1:B:1792:ARG:HH21	1:B:1860:ARG:NE	2.19	0.41
1:A:1387:LYS:HG3	1:A:1427:LEU:HD13	2.02	0.41
1:A:2335:ILE:HG23	1:A:2335:ILE:O	2.21	0.41
1:A:2397:TYR:HA	1:A:2472:LEU:HD21	2.02	0.41
1:A:798:LYS:HG2	1:A:810:ARG:NE	2.35	0.41
1:A:1814:GLU:HA	1:A:1817:VAL:HG12	2.03	0.41
1:B:288:ARG:HA	1:B:291:HIS:HD2	1.84	0.41
1:B:2335:ILE:HG23	1:B:2335:ILE:O	2.21	0.41
1:A:237:PHE:O	1:A:241:VAL:HG23	2.20	0.41
1:A:685:ARG:HA	1:A:688:LYS:CE	2.48	0.41
1:A:2267:ASP:HB2	1:A:2330:LYS:NZ	2.36	0.41
1:B:82:LYS:HZ1	1:B:84:SER:HB3	1.82	0.41
1:B:112:PHE:CE1	1:B:134:VAL:HG22	2.56	0.41
1:B:310:LEU:HD12	1:B:313:LYS:HD2	2.03	0.41
1:B:895:VAL:HG12	1:B:897:GLU:H	1.86	0.41
1:B:928:LEU:HD22	1:B:968:PHE:HD1	1.85	0.41
1:A:1089:GLY:HA3	1:A:1134:LEU:HD21	2.02	0.41
1:A:2030:LEU:CG	1:A:2034:LYS:HE3	2.48	0.41
1:B:140:LYS:HB2	1:B:147:ILE:HD13	2.03	0.41
1:B:685:ARG:HA	1:B:688:LYS:CE	2.49	0.41
1:B:844:ASN:HD21	1:B:901:LYS:HZ2	1.67	0.41
1:B:1302:ALA:HA	1:B:1361:ILE:HG21	2.02	0.41
1:B:1811:PHE:HA	1:B:1814:GLU:HG2	2.03	0.41
1:A:594:LEU:HD22	1:A:613:LEU:HD22	2.02	0.41
1:A:798:LYS:CE	1:A:810:ARG:HE	2.21	0.41
1:A:1128:LYS:HE2	1:A:1263:MET:HE3	2.02	0.41
1:B:85:ASP:O	1:B:89:VAL:HG12	2.21	0.41
1:B:231:ILE:HG21	1:B:273:MET:HA	2.03	0.41
1:B:1404:ASN:HD22	1:B:1404:ASN:HA	1.78	0.40
1:B:2003:MET:HE2	1:B:2003:MET:HB3	1.96	0.40
1:B:2051:ILE:O	1:B:2055:ILE:HG13	2.20	0.40
1:A:479:TYR:HD2	1:A:490:ILE:HD11	1.86	0.40
1:A:799:THR:HG22	1:A:810:ARG:HD2	2.03	0.40
1:B:1:MET:HE1	1:B:50:LEU:HD22	2.02	0.40
1:B:2267:ASP:HB2	1:B:2330:LYS:NZ	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2351:ASP:HB3	1:B:2354:MET:HB2	2.03	0.40
1:A:162:LEU:HD23	1:A:215:HIS:ND1	2.36	0.40
1:A:844:ASN:ND2	1:A:901:LYS:NZ	2.69	0.40
1:A:2359:ASN:HB3	1:A:2362:GLU:H	1.86	0.40
1:A:2474:LYS:HD3	1:A:2474:LYS:HA	1.83	0.40
1:B:591:MET:HE1	1:B:637:LEU:HD23	2.04	0.40
1:B:844:ASN:HD21	1:B:901:LYS:NZ	2.19	0.40
1:B:1387:LYS:HG3	1:B:1427:LEU:HD13	2.02	0.40
1:B:1814:GLU:HA	1:B:1817:VAL:HG12	2.03	0.40
1:B:2136:ILE:HG12	1:B:2164:ALA:HB1	2.04	0.40
1:A:1:MET:SD	1:A:54:VAL:HG12	2.62	0.40
1:A:841:MET:HG2	1:A:905:ILE:HD11	2.03	0.40
1:A:1404:ASN:HD22	1:A:1404:ASN:HA	1.76	0.40
1:B:621:VAL:HB	1:B:632:THR:HG22	2.03	0.40
1:B:850:MET:HA	1:B:912:ILE:HG12	2.03	0.40
1:B:1825:VAL:HG23	1:B:1826:GLU:HG3	2.03	0.40
1:A:473:PHE:CD1	1:A:520:LEU:HD22	2.56	0.40
1:A:525:PHE:HE1	1:A:534:ILE:HG21	1.87	0.40
1:A:1779:VAL:CG2	1:A:1811:PHE:HD2	2.34	0.40
1:B:1251:PHE:HD2	1:B:1275:LEU:HD13	1.86	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	2129/2492 (85%)	2019 (95%)	106 (5%)	4 (0%)	43	73
1	B	2128/2492 (85%)	2011 (94%)	112 (5%)	5 (0%)	43	73
All	All	4257/4984 (85%)	4030 (95%)	218 (5%)	9 (0%)	43	73

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1064	THR
1	B	1064	THR
1	A	170	PRO
1	A	2481	GLU
1	B	170	PRO
1	B	1168	TYR
1	B	1207	ARG
1	B	243	TYR
1	A	243	TYR

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	1955/2267 (86%)	1843 (94%)	112 (6%)	18	49
1	B	1955/2267 (86%)	1852 (95%)	103 (5%)	20	51
All	All	3910/4534 (86%)	3695 (94%)	215 (6%)	19	50

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	89	VAL
1	A	99	LEU
1	A	112	PHE
1	A	113	ASP
1	A	124	LEU
1	A	137	PHE
1	A	147	ILE
1	A	166	VAL
1	A	224	GLU
1	A	225	GLN
1	A	229	LEU
1	A	250	ILE
1	A	253	GLU
1	A	257	ARG

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Mol	Chain	Res	Type
1	A	263	LEU
1	A	272	GLN
1	A	306	MET
1	A	310	LEU
1	A	326	VAL
1	A	382	LEU
1	A	395	ILE
1	A	434	LYS
1	A	446	LEU
1	A	461	SER
1	A	462	GLU
1	A	465	THR
1	A	529	GLU
1	A	560	ASP
1	A	579	ILE
1	A	594	LEU
1	A	619	ARG
1	A	626	THR
1	A	679	ILE
1	A	681	LYS
1	A	688	LYS
1	A	718	GLU
1	A	747	THR
1	A	769	ILE
1	A	779	THR
1	A	800	GLU
1	A	857	VAL
1	A	920	ILE
1	A	928	LEU
1	A	940	LEU
1	A	945	THR
1	A	971	VAL
1	A	993	VAL
1	A	994	LYS
1	A	997	LYS
1	A	1010	LEU
1	A	1055	VAL
1	A	1075	VAL
1	A	1108	ILE
1	A	1113	ILE
1	A	1122	VAL
1	A	1166	ARG

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Mol	Chain	Res	Type
1	A	1206	ILE
1	A	1316	GLU
1	A	1320	LEU
1	A	1373	ARG
1	A	1375	SER
1	A	1402	ILE
1	A	1403	ASP
1	A	1404	ASN
1	A	1405	ARG
1	A	1411	SER
1	A	1431	GLU
1	A	1537	LEU
1	A	1539	ILE
1	A	1549	GLU
1	A	1550	MET
1	A	1562	VAL
1	A	1574	LEU
1	A	1779	VAL
1	A	1786	VAL
1	A	1825	VAL
1	A	1852	ILE
1	A	1857	ILE
1	A	1925	VAL
1	A	1974	CYS
1	A	1975	LEU
1	A	2005	ILE
1	A	2008	THR
1	A	2052	VAL
1	A	2059	ILE
1	A	2070	GLU
1	A	2083	VAL
1	A	2084	GLU
1	A	2099	ASP
1	A	2105	PHE
1	A	2130	VAL
1	A	2131	GLN
1	A	2138	LEU
1	A	2204	ILE
1	A	2216	ILE
1	A	2217	ASN
1	A	2247	ARG
1	A	2286	LEU

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Mol	Chain	Res	Type
1	A	2317	GLU
1	A	2325	LEU
1	A	2331	LEU
1	A	2335	ILE
1	A	2349	ILE
1	A	2355	LEU
1	A	2368	SER
1	A	2425	GLU
1	A	2433	GLN
1	A	2458	PHE
1	A	2470	GLU
1	A	2479	SER
1	A	2480	LEU
1	B	89	VAL
1	B	99	LEU
1	B	112	PHE
1	B	113	ASP
1	B	137	PHE
1	B	145	ARG
1	B	166	VAL
1	B	189	ILE
1	B	227	GLU
1	B	250	ILE
1	B	253	GLU
1	B	257	ARG
1	B	272	GLN
1	B	288	ARG
1	B	289	ILE
1	B	306	MET
1	B	310	LEU
1	B	326	VAL
1	B	341	VAL
1	B	382	LEU
1	B	395	ILE
1	B	434	LYS
1	B	446	LEU
1	B	455	SER
1	B	461	SER
1	B	462	GLU
1	B	465	THR
1	B	512	ASP
1	B	528	SER

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Mol	Chain	Res	Type
1	B	529	GLU
1	B	594	LEU
1	B	626	THR
1	B	679	ILE
1	B	688	LYS
1	B	718	GLU
1	B	750	VAL
1	B	779	THR
1	B	857	VAL
1	B	899	LYS
1	B	900	LYS
1	B	928	LEU
1	B	940	LEU
1	B	945	THR
1	B	971	VAL
1	B	1010	LEU
1	B	1055	VAL
1	B	1075	VAL
1	B	1108	ILE
1	B	1122	VAL
1	B	1166	ARG
1	B	1168	TYR
1	B	1198	CYS
1	B	1206	ILE
1	B	1257	HIS
1	B	1316	GLU
1	B	1320	LEU
1	B	1330	LEU
1	B	1373	ARG
1	B	1403	ASP
1	B	1404	ASN
1	B	1405	ARG
1	B	1439	VAL
1	B	1537	LEU
1	B	1539	ILE
1	B	1549	GLU
1	B	1562	VAL
1	B	1574	LEU
1	B	1779	VAL
1	B	1786	VAL
1	B	1825	VAL
1	B	1852	ILE

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Mol	Chain	Res	Type
1	B	1857	ILE
1	B	1925	VAL
1	B	1953	ARG
1	B	1961	LEU
1	B	1974	CYS
1	B	1975	LEU
1	B	2005	ILE
1	B	2059	ILE
1	B	2070	GLU
1	B	2083	VAL
1	B	2084	GLU
1	B	2086	GLU
1	B	2099	ASP
1	B	2130	VAL
1	B	2131	GLN
1	B	2138	LEU
1	B	2204	ILE
1	B	2216	ILE
1	B	2217	ASN
1	B	2325	LEU
1	B	2331	LEU
1	B	2335	ILE
1	B	2339	LEU
1	B	2349	ILE
1	B	2355	LEU
1	B	2359	ASN
1	B	2368	SER
1	B	2425	GLU
1	B	2433	GLN
1	B	2458	PHE
1	B	2470	GLU
1	B	2479	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	182	ASN
1	A	225	GLN
1	A	244	ASN
1	A	267	ASN
1	A	291	HIS

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Mol	Chain	Res	Type
1	A	322	HIS
1	A	355	ASN
1	A	360	GLN
1	A	412	ASN
1	A	416	HIS
1	A	423	ASN
1	A	435	ASN
1	A	481	HIS
1	A	519	ASN
1	A	527	ASN
1	A	593	ASN
1	A	628	ASN
1	A	672	GLN
1	A	713	ASN
1	A	723	HIS
1	A	731	GLN
1	A	755	ASN
1	A	801	GLN
1	A	804	HIS
1	A	809	GLN
1	A	844	ASN
1	A	852	HIS
1	A	890	ASN
1	A	908	HIS
1	A	927	HIS
1	A	974	ASN
1	A	995	ASN
1	A	1001	GLN
1	A	1012	GLN
1	A	1024	HIS
1	A	1088	GLN
1	A	1103	ASN
1	A	1136	ASN
1	A	1161	HIS
1	A	1247	ASN
1	A	1334	HIS
1	A	1367	GLN
1	A	1404	ASN
1	A	1527	GLN
1	A	1794	ASN
1	A	1801	ASN
1	A	1882	ASN

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Mol	Chain	Res	Type
1	A	1922	ASN
1	A	1982	ASN
1	A	2091	ASN
1	A	2109	GLN
1	A	2131	GLN
1	A	2141	GLN
1	A	2151	HIS
1	A	2152	GLN
1	A	2197	ASN
1	A	2209	GLN
1	A	2280	ASN
1	A	2318	ASN
1	A	2381	ASN
1	A	2392	GLN
1	A	2414	GLN
1	A	2434	ASN
1	A	2455	HIS
1	B	142	HIS
1	B	225	GLN
1	B	244	ASN
1	B	291	HIS
1	B	322	HIS
1	B	355	ASN
1	B	360	GLN
1	B	412	ASN
1	B	416	HIS
1	B	423	ASN
1	B	435	ASN
1	B	481	HIS
1	B	519	ASN
1	B	593	ASN
1	B	628	ASN
1	B	672	GLN
1	B	713	ASN
1	B	723	HIS
1	B	731	GLN
1	B	755	ASN
1	B	801	GLN
1	B	809	GLN
1	B	831	ASN
1	B	844	ASN
1	B	852	HIS

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Mol	Chain	Res	Type
1	B	890	ASN
1	B	908	HIS
1	B	927	HIS
1	B	974	ASN
1	B	1001	GLN
1	B	1024	HIS
1	B	1088	GLN
1	B	1103	ASN
1	B	1136	ASN
1	B	1161	HIS
1	B	1208	HIS
1	B	1247	ASN
1	B	1334	HIS
1	B	1367	GLN
1	B	1404	ASN
1	B	1563	GLN
1	B	1801	ASN
1	B	1882	ASN
1	B	1922	ASN
1	B	1982	ASN
1	B	2053	HIS
1	B	2103	HIS
1	B	2109	GLN
1	B	2141	GLN
1	B	2151	HIS
1	B	2152	GLN
1	B	2197	ASN
1	B	2209	GLN
1	B	2244	HIS
1	B	2280	ASN
1	B	2359	ASN
1	B	2381	ASN
1	B	2392	GLN
1	B	2414	GLN
1	B	2434	ASN

5.3.3 RNA ⓘ

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 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

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	2143/2492 (85%)	0.14	37 (1%) 69 45	45, 101, 157, 222	0
1	B	2144/2492 (86%)	0.14	41 (1%) 66 42	44, 105, 152, 223	0
All	All	4287/4984 (86%)	0.14	78 (1%) 67 43	44, 103, 155, 223	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	ILE	5.6
1	B	954	GLY	5.1
1	B	2445	SER	4.6
1	A	189	ILE	3.9
1	A	198	TYR	3.7
1	A	289	ILE	3.7
1	B	197	ILE	3.7
1	B	213	PHE	3.5
1	A	196	GLY	3.4
1	A	14	PRO	3.4
1	B	188	SER	3.4
1	B	1254	LEU	3.4
1	A	2059	ILE	3.4
1	B	289	ILE	3.3
1	A	2064	ASN	3.2
1	A	213	PHE	3.2
1	B	2332	VAL	3.1
1	A	2284	ASN	3.0
1	B	195	LYS	3.0
1	B	198	TYR	3.0
1	A	246	THR	2.9
1	B	1185	ILE	2.9
1	B	1206	ILE	2.8
1	A	911	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1201	ALA	2.8
1	B	80	PRO	2.8
1	B	2300	THR	2.7
1	A	2332	VAL	2.7
1	A	195	LYS	2.7
1	B	1574	LEU	2.6
1	A	163	ILE	2.6
1	B	206	PRO	2.6
1	B	196	GLY	2.6
1	A	192	ALA	2.6
1	B	404	LEU	2.5
1	B	802	ILE	2.5
1	A	828	PRO	2.5
1	B	2286	LEU	2.5
1	A	1311	SER	2.4
1	A	328	PHE	2.4
1	B	1162	LEU	2.4
1	A	450	PHE	2.4
1	B	1568	GLY	2.4
1	B	137	PHE	2.4
1	A	2069	SER	2.4
1	A	1206	ILE	2.4
1	A	1160	LYS	2.4
1	B	1540	LEU	2.3
1	A	-1	GLY	2.3
1	B	143	ILE	2.3
1	A	43	TRP	2.3
1	A	2285	VAL	2.3
1	B	1197	GLU	2.2
1	B	2175	GLY	2.2
1	B	74	GLY	2.2
1	B	690	LYS	2.2
1	B	1553	PHE	2.2
1	A	1308	LEU	2.2
1	A	1976	ASP	2.2
1	B	1308	LEU	2.2
1	A	1440	THR	2.2
1	B	176	TYR	2.2
1	A	193	VAL	2.2
1	B	968	PHE	2.2
1	A	895	VAL	2.2
1	B	2059	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1000	LYS	2.2
1	A	74	GLY	2.1
1	B	525	PHE	2.1
1	A	309	ASN	2.1
1	B	250	ILE	2.1
1	B	1240	ILE	2.1
1	B	199	SER	2.1
1	A	690	LYS	2.0
1	B	475	ALA	2.0
1	B	887	GLY	2.0
1	A	218	ARG	2.0
1	A	804	HIS	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.