



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 07:23 am GMT

PDB ID : 2X6H
Title : THE CRYSTAL STRUCTURE OF THE DROSOPHILA CLASS III PI3-KINASE VPS34
Authors : Miller, S.; Tavshanjian, B.; Oleksy, A.; Perisic, O.; Houseman, B.T.; Shokat, K.M.; Williams, R.L.
Deposited on : 2010-02-17
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

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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

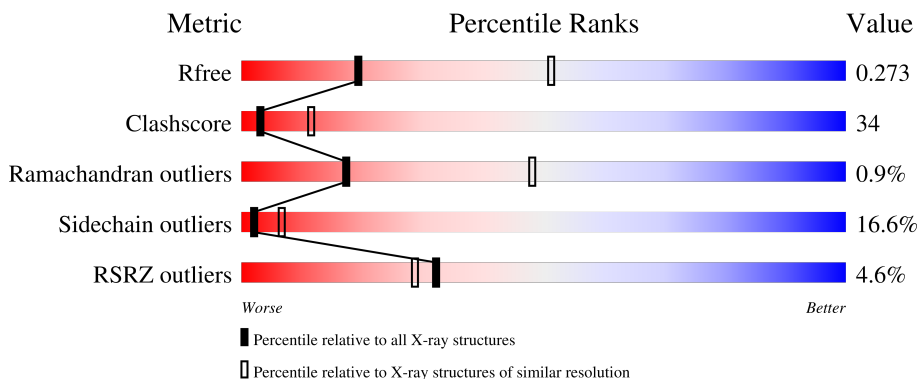
1 Overall quality at a glance

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 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	696	 3% 41% 28% 8% • 22%
1	B	696	 4% 38% 33% 7% • 22%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8916 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 PHOSPHOTIDYLINOSITOL 3 KINASE 59F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	543	4445	2874	755	789	27	0	0	0
1	B	543	4441	2870	759	785	27	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	expression tag	UNP Q9W1M7
A	255	SER	-	expression tag	UNP Q9W1M7
A	256	HIS	-	expression tag	UNP Q9W1M7
A	257	MET	-	expression tag	UNP Q9W1M7
A	455	ALA	GLY	engineered mutation	UNP Q9W1M7
B	254	GLY	-	expression tag	UNP Q9W1M7
B	255	SER	-	expression tag	UNP Q9W1M7
B	256	HIS	-	expression tag	UNP Q9W1M7
B	257	MET	-	expression tag	UNP Q9W1M7
B	455	ALA	GLY	engineered mutation	UNP Q9W1M7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	11	Total	O	0	0
			11	11		

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.60Å 154.79Å 243.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.36 – 2.90 72.32 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (72.36-2.90) 95.6 (72.32-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.240 , 0.278 0.236 , 0.273	Depositor DCC
R_{free} test set	2228 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	76.2	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8916	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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	0.61	2/4553 (0.0%)	0.86	3/6164 (0.0%)
1	B	0.47	0/4548	0.68	6/6156 (0.1%)
All	All	0.55	2/9101 (0.0%)	0.78	9/12320 (0.1%)

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	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	750	CYS	CB-SG	-5.59	1.72	1.81
1	A	791	CYS	CB-SG	-5.37	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	LEU	CA-CB-CG	6.42	130.06	115.30
1	B	722	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	710	LEU	CA-CB-CG	-6.25	100.92	115.30
1	A	710	LEU	CA-CB-CG	-5.88	101.77	115.30
1	B	343	LEU	CA-CB-CG	5.49	127.92	115.30
1	B	614	LEU	CA-CB-CG	5.40	127.72	115.30
1	B	351	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	836	PRO	C-N-CD	-5.16	109.25	120.60
1	B	398	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	590	GLY	Mainchain
1	A	591	ASN	Mainchain
1	A	737	THR	Mainchain
1	A	835	MET	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	4445	0	4478	273	1
1	B	4441	0	4485	337	0
2	A	19	0	0	4	0
2	B	11	0	0	0	0
All	All	8916	0	8963	603	1

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 34.

All (603) 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:602:ARG:HD2	1:A:606:ARG:NH1	1.38	1.34
1:A:335:PHE:CE2	1:A:339:ILE:HD11	1.70	1.27
1:A:322:ARG:NH2	1:A:338:CYS:SG	2.11	1.22
1:A:335:PHE:HD1	1:A:357:TRP:CZ3	1.58	1.21
1:A:335:PHE:CD1	1:A:357:TRP:CZ3	2.30	1.19
1:B:669:ARG:NH1	1:B:683:THR:OG1	1.84	1.10
1:B:738:SER:HB3	1:B:741:HIS:CE1	1.86	1.10
1:B:315:GLN:HB2	1:B:338:CYS:HB3	1.31	1.10
1:A:335:PHE:CD1	1:A:357:TRP:HZ3	1.65	1.09
1:B:354:LEU:HD21	1:B:381:TYR:CD1	1.88	1.07
1:A:409:ASP:HB2	1:A:412:HIS:CD2	1.90	1.06
1:A:319:TRP:HA	1:A:322:ARG:HD2	1.39	1.04
1:A:669:ARG:HD3	2:A:2009:HOH:O	1.57	1.04
1:B:300:ILE:HA	1:B:304:TYR:CE2	1.92	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:PHE:CD2	1:A:339:ILE:HD11	1.94	1.03
1:A:306:PRO:HD2	1:A:308:TYR:CE2	1.95	1.02
1:A:602:ARG:CD	1:A:606:ARG:HH12	1.75	0.99
1:A:409:ASP:HB2	1:A:412:HIS:NE2	1.76	0.99
1:A:291:ALA:HB3	1:A:294:ARG:HB2	1.45	0.99
1:A:335:PHE:HE2	1:A:339:ILE:HD11	1.20	0.98
1:A:577:ALA:O	1:A:581:LYS:HD2	1.64	0.97
1:A:602:ARG:CD	1:A:606:ARG:NH1	2.30	0.94
1:B:739:SER:O	1:B:740:LYS:HG2	1.67	0.94
1:B:639:GLN:HE21	1:B:645:ASN:HD21	1.11	0.94
1:B:738:SER:HB3	1:B:741:HIS:HE1	1.30	0.92
1:B:837:PRO:O	1:B:840:LYS:HE2	1.70	0.92
1:B:300:ILE:HA	1:B:304:TYR:HE2	1.28	0.91
1:B:375:HIS:CD2	1:B:377:GLN:H	1.89	0.91
1:A:734:VAL:HG22	1:A:744:LEU:HD23	1.52	0.91
1:B:297:LEU:O	1:B:300:ILE:HG22	1.71	0.91
1:B:300:ILE:O	1:B:304:TYR:HD2	1.53	0.91
1:B:322:ARG:HH22	1:B:334:LYS:HB2	1.35	0.91
1:A:806:ARG:NH2	1:A:822:ILE:O	2.03	0.90
1:B:639:GLN:NE2	1:B:645:ASN:HD21	1.67	0.90
1:A:306:PRO:HD2	1:A:308:TYR:CD2	2.06	0.90
1:A:319:TRP:HA	1:A:322:ARG:CD	2.03	0.88
1:B:375:HIS:HD2	1:B:377:GLN:H	1.15	0.88
1:B:300:ILE:O	1:B:304:TYR:CD2	2.26	0.87
1:B:782:GLU:O	1:B:786:THR:HG22	1.73	0.87
1:A:608:ILE:O	1:A:612:VAL:HG23	1.73	0.87
1:B:836:PRO:HB2	1:B:837:PRO:HA	1.57	0.86
1:B:417:HIS:ND1	1:B:578:MET:HG3	1.90	0.85
1:A:335:PHE:HE2	1:A:339:ILE:CD1	1.88	0.85
1:B:633:GLN:NE2	1:B:668:MET:SD	2.50	0.85
1:A:367:GLU:O	1:A:370:SER:HB3	1.75	0.84
1:B:339:ILE:HD13	1:B:350:ALA:CB	2.08	0.84
1:A:625:ARG:O	1:A:629:THR:HG22	1.78	0.84
1:B:339:ILE:HD13	1:B:350:ALA:HB1	1.60	0.84
1:B:639:GLN:HE21	1:B:645:ASN:ND2	1.75	0.84
1:B:315:GLN:CB	1:B:338:CYS:HB3	2.06	0.83
1:B:751:THR:HG22	1:B:754:GLU:H	1.44	0.82
1:A:320:LYS:HG3	1:A:321:PHE:HD2	1.42	0.82
1:A:335:PHE:HD1	1:A:357:TRP:CH2	1.97	0.82
1:B:776:PRO:HB2	1:B:777:TYR:HD1	1.45	0.81
1:B:710:LEU:HD22	1:B:732:TYR:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ILE:HG21	1:A:350:ALA:CB	2.11	0.81
1:B:575:MET:HE2	1:B:576:TYR:HD2	1.45	0.81
1:B:329:LYS:HD3	1:B:361:ASP:OD1	1.80	0.81
1:B:812:LEU:HD22	1:B:812:LEU:N	1.96	0.81
1:B:648:ASN:HA	1:B:664:LYS:HB3	1.63	0.80
1:A:674:LYS:H	1:A:674:LYS:HD3	1.45	0.79
1:A:335:PHE:CE2	1:A:339:ILE:CD1	2.58	0.79
1:A:602:ARG:HD2	1:A:606:ARG:HH12	0.80	0.79
1:A:323:PHE:HZ	1:A:349:GLN:HE22	1.32	0.78
1:B:763:HIS:CE1	1:B:777:TYR:CD2	2.71	0.78
1:B:667:PRO:O	1:B:670:THR:HG23	1.84	0.78
1:B:830:ARG:HH22	1:B:903:LYS:HZ2	1.31	0.78
1:B:888:ALA:O	1:B:889:THR:HG22	1.82	0.78
1:B:311:SER:O	1:B:315:GLN:N	2.16	0.77
1:B:315:GLN:HB2	1:B:338:CYS:CB	2.10	0.77
1:B:763:HIS:HE1	1:B:777:TYR:CD2	2.01	0.77
1:A:798:THR:HG23	1:A:803:VAL:HB	1.66	0.77
1:A:922:GLN:HE22	1:B:919:GLN:HB3	1.50	0.77
1:B:639:GLN:NE2	1:B:647:THR:OG1	2.18	0.77
1:B:824:PHE:HB3	1:B:827:ILE:HD11	1.65	0.77
1:A:306:PRO:CD	1:A:308:TYR:CE2	2.67	0.77
1:B:360:MET:HG2	1:B:364:ASP:HB2	1.65	0.77
1:A:827:ILE:HG23	1:A:828:LEU:HG	1.65	0.76
1:A:307:THR:OG1	1:A:905:GLU:OE2	2.03	0.76
1:A:717:ASP:OD2	1:A:721:ARG:NH1	2.19	0.76
1:B:398:LEU:HA	1:B:401:LEU:HB2	1.68	0.76
1:B:577:ALA:O	1:B:581:LYS:HD3	1.86	0.76
1:A:710:LEU:HD23	1:A:732:TYR:O	1.85	0.75
1:B:311:SER:HA	1:B:314:GLU:HB2	1.68	0.75
1:B:311:SER:HA	1:B:314:GLU:CD	2.07	0.75
1:B:798:THR:HG23	1:B:803:VAL:HB	1.68	0.75
1:B:876:ASN:ND2	1:B:876:ASN:H	1.82	0.75
1:A:320:LYS:HG3	1:A:321:PHE:CD2	2.21	0.75
1:A:299:THR:HA	1:A:302:TYR:HD2	1.52	0.74
1:B:836:PRO:HB2	1:B:837:PRO:CA	2.17	0.74
1:A:412:HIS:CD2	1:A:412:HIS:H	2.05	0.74
1:A:677:LEU:O	1:A:679:PRO:HD3	1.87	0.74
1:B:667:PRO:O	1:B:670:THR:CG2	2.35	0.74
1:A:339:ILE:HG21	1:A:350:ALA:HB2	1.68	0.74
1:A:608:ILE:HG21	1:A:737:THR:HG21	1.68	0.73
1:A:861:ARG:NH2	1:A:926:ASP:OD2	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:LEU:HB3	1:A:581:LYS:HE3	1.70	0.73
1:B:363:GLU:HG2	1:B:877:VAL:HG22	1.70	0.73
1:B:416:LEU:HB3	1:B:582:MET:HE1	1.70	0.73
1:A:294:ARG:NH2	1:A:298:HIS:NE2	2.36	0.73
1:B:306:PRO:HG2	1:B:879:LEU:HD12	1.70	0.73
1:B:751:THR:CG2	1:B:754:GLU:H	2.02	0.73
1:B:329:LYS:HG2	1:B:359:PRO:O	1.87	0.73
1:B:575:MET:HE2	1:B:576:TYR:CD2	2.24	0.72
1:A:872:ARG:NH1	1:A:909:GLN:O	2.22	0.72
1:B:302:TYR:CE1	1:B:331:ALA:HB2	2.24	0.72
1:A:295:ASP:O	1:A:299:THR:HG23	1.90	0.71
1:A:306:PRO:HD2	1:A:308:TYR:HE2	1.51	0.71
1:A:306:PRO:CD	1:A:308:TYR:HE2	2.04	0.71
1:A:318:VAL:O	1:A:322:ARG:HG3	1.91	0.71
1:A:835:MET:HB3	1:A:836:PRO:O	1.91	0.71
1:A:930:THR:HG22	1:A:936:LEU:HB3	1.73	0.71
1:B:354:LEU:HD21	1:B:381:TYR:CE1	2.26	0.70
1:A:931:ALA:O	1:B:944:THR:OG1	2.09	0.70
1:B:416:LEU:HD22	1:B:535:THR:HG22	1.73	0.70
1:B:577:ALA:O	1:B:581:LYS:CD	2.39	0.70
1:A:669:ARG:CD	2:A:2009:HOH:O	2.28	0.70
1:A:926:ASP:O	1:A:930:THR:OG1	2.09	0.70
1:B:830:ARG:NH2	1:B:903:LYS:HZ2	1.89	0.70
1:B:302:TYR:HE1	1:B:331:ALA:HB2	1.55	0.70
1:B:722:ARG:HH11	1:B:722:ARG:HA	1.55	0.70
1:A:552:TYR:C	1:A:552:TYR:CD2	2.65	0.70
1:A:709:ILE:HG13	1:A:827:ILE:HD11	1.75	0.69
1:A:314:GLU:HA	1:A:317:LEU:HG	1.75	0.69
1:B:722:ARG:HH11	1:B:722:ARG:CA	2.04	0.69
1:B:812:LEU:HD22	1:B:812:LEU:H	1.58	0.69
1:A:314:GLU:O	1:A:318:VAL:HG23	1.93	0.69
1:A:335:PHE:CE1	1:A:357:TRP:HZ3	2.09	0.69
1:B:634:LYS:HA	1:B:634:LYS:HE2	1.74	0.69
1:B:664:LYS:HG3	1:B:685:VAL:CG2	2.24	0.68
1:A:866:THR:O	1:A:870:HIS:HD2	1.76	0.68
1:A:291:ALA:HB3	1:A:294:ARG:CB	2.21	0.68
1:B:703:LEU:HB2	1:B:736:ALA:HB2	1.76	0.68
1:B:391:ASP:OD2	1:B:540:ARG:NH2	2.27	0.68
1:A:629:THR:HB	1:A:672:LEU:HG	1.76	0.67
1:A:677:LEU:HD22	1:A:700:GLY:HA3	1.76	0.67
1:B:354:LEU:HD21	1:B:381:TYR:HD1	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:GLN:HE22	1:B:711:GLN:HE22	1.42	0.67
1:B:331:ALA:HB1	1:B:357:TRP:HZ2	1.60	0.67
1:B:360:MET:HE2	1:B:381:TYR:HE2	1.59	0.67
1:A:909:GLN:HA	1:A:909:GLN:OE1	1.93	0.67
1:A:806:ARG:HD2	1:A:806:ARG:N	2.09	0.67
1:A:913:THR:HG23	1:A:916:GLU:HB2	1.76	0.67
1:B:843:LYS:HA	1:B:932:VAL:CG1	2.25	0.67
1:B:322:ARG:HH22	1:B:334:LYS:CB	2.08	0.67
1:B:370:SER:OG	1:B:372:THR:HG23	1.94	0.66
1:A:352:TRP:O	1:A:356:ASN:ND2	2.28	0.66
1:B:360:MET:CG	1:B:364:ASP:HB2	2.26	0.66
1:B:664:LYS:CG	1:B:685:VAL:CG2	2.74	0.66
1:B:776:PRO:HD2	1:B:779:ILE:O	1.94	0.66
1:A:573:HIS:C	1:A:573:HIS:CD2	2.69	0.66
1:A:373:PHE:N	1:A:373:PHE:HD2	1.94	0.66
1:B:876:ASN:H	1:B:876:ASN:HD22	1.43	0.66
1:A:777:TYR:HB2	1:A:779:ILE:HD12	1.78	0.66
1:A:948:ARG:HD2	1:A:948:ARG:C	2.16	0.65
1:B:716:MET:HG2	1:B:878:MET:CE	2.26	0.65
1:A:300:ILE:O	1:A:304:TYR:HB2	1.96	0.65
1:B:863:GLN:O	1:B:866:THR:HG22	1.96	0.65
1:B:764:ASN:OD1	1:B:767:ARG:NH1	2.29	0.65
1:A:409:ASP:CB	1:A:412:HIS:CD2	2.73	0.65
1:B:654:PHE:HD1	1:B:655:PRO:HD2	1.61	0.65
1:A:335:PHE:HD2	1:A:335:PHE:C	1.99	0.65
1:A:737:THR:HG22	1:A:738:SER:H	1.61	0.65
1:B:354:LEU:C	1:B:354:LEU:HD23	2.17	0.65
1:A:306:PRO:CD	1:A:308:TYR:CD2	2.80	0.64
1:B:553:TRP:O	1:B:557:ILE:HG13	1.96	0.64
1:B:698:LYS:O	1:B:741:HIS:HA	1.97	0.64
1:B:751:THR:HG22	1:B:754:GLU:CB	2.27	0.64
1:B:830:ARG:HH22	1:B:903:LYS:NZ	1.95	0.64
1:A:335:PHE:CD2	1:A:335:PHE:C	2.71	0.64
1:A:737:THR:HG22	1:A:738:SER:N	2.13	0.64
1:B:733:LYS:H	1:B:745:GLN:HE21	1.45	0.64
1:A:405:LEU:HD23	1:A:533:LEU:CD2	2.26	0.64
1:B:751:THR:HG22	1:B:754:GLU:HB2	1.80	0.64
1:B:830:ARG:HH12	1:B:903:LYS:HZ2	1.46	0.63
1:B:836:PRO:CB	1:B:837:PRO:CA	2.76	0.63
1:B:375:HIS:HD2	1:B:377:GLN:N	1.93	0.63
1:A:323:PHE:CE1	1:A:349:GLN:OE1	2.50	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ARG:O	1:A:629:THR:CG2	2.46	0.63
1:B:669:ARG:HH11	1:B:683:THR:HG1	1.43	0.63
1:A:656:LEU:HD22	1:A:733:LYS:HB3	1.81	0.63
1:B:314:GLU:O	1:B:317:LEU:HG	1.99	0.63
1:B:360:MET:HE2	1:B:381:TYR:CE2	2.35	0.62
1:B:417:HIS:ND1	1:B:578:MET:CG	2.61	0.62
1:A:412:HIS:H	1:A:412:HIS:HD2	1.45	0.62
1:B:318:VAL:O	1:B:322:ARG:HG3	2.00	0.62
1:A:400:GLN:HG2	1:A:881:LEU:HD22	1.82	0.62
1:A:575:MET:O	1:A:579:VAL:HG23	1.99	0.61
1:A:409:ASP:HB2	1:A:412:HIS:HE2	1.61	0.61
1:A:373:PHE:N	1:A:373:PHE:CD2	2.66	0.61
1:B:568:GLN:OE1	1:B:568:GLN:HA	1.99	0.61
1:A:710:LEU:CD2	1:A:732:TYR:O	2.48	0.61
1:B:777:TYR:HB2	1:B:779:ILE:HD12	1.83	0.61
1:A:942:ARG:HD3	1:B:835:MET:HG3	1.82	0.61
1:A:553:TRP:O	1:A:557:ILE:HG13	2.01	0.60
1:A:888:ALA:O	1:A:889:THR:HG23	2.01	0.60
1:B:810:ASN:O	1:B:822:ILE:HG22	2.02	0.60
1:A:674:LYS:HD3	1:A:674:LYS:N	2.16	0.60
1:B:823:ASP:OD1	1:B:823:ASP:C	2.40	0.60
1:B:557:ILE:O	1:B:560:GLU:HG2	2.02	0.60
1:A:751:THR:HG23	1:A:754:GLU:CG	2.31	0.60
1:B:363:GLU:HG3	1:B:877:VAL:HG13	1.83	0.60
1:A:294:ARG:HH22	1:A:317:LEU:HB2	1.66	0.60
1:B:898:ASP:OD1	1:B:898:ASP:N	2.34	0.60
1:B:319:TRP:NE1	1:B:323:PHE:CZ	2.69	0.60
1:B:664:LYS:CG	1:B:685:VAL:HG21	2.32	0.59
1:B:780:SER:HB3	1:B:782:GLU:OE2	2.02	0.59
1:A:313:GLU:CA	1:A:313:GLU:OE1	2.49	0.59
1:A:629:THR:O	1:A:633:GLN:HG3	2.02	0.59
1:B:812:LEU:N	1:B:812:LEU:CD2	2.65	0.59
1:A:322:ARG:HH22	1:A:338:CYS:HG	1.43	0.59
1:A:674:LYS:H	1:A:674:LYS:CD	2.09	0.59
1:B:830:ARG:NH1	1:B:903:LYS:HZ2	2.00	0.59
1:A:322:ARG:HH12	1:A:338:CYS:HB2	1.68	0.59
1:A:813:LEU:HD12	1:A:818:LYS:O	2.02	0.59
1:B:348:THR:HA	1:B:351:LEU:HD22	1.83	0.59
1:B:370:SER:HB2	1:B:371:PRO:CD	2.33	0.59
1:B:636:LEU:CD1	1:B:670:THR:HG21	2.33	0.59
1:B:677:LEU:O	1:B:679:PRO:HD3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:768:LYS:HB3	1:B:769:HIS:HD2	1.68	0.58
1:A:827:ILE:HG22	1:A:892:ASP:CB	2.32	0.58
1:A:739:SER:O	1:A:740:LYS:HG2	2.03	0.58
1:B:320:LYS:HG3	1:B:321:PHE:N	2.19	0.58
1:B:541:ALA:O	1:B:548:ALA:HB2	2.03	0.58
1:A:772:CYS:O	1:A:778:GLY:HA2	2.03	0.58
1:B:322:ARG:HD3	1:B:335:PHE:CD1	2.39	0.58
1:B:909:GLN:HG3	1:B:912:LEU:HG	1.85	0.58
1:B:639:GLN:NE2	1:B:645:ASN:ND2	2.43	0.58
1:B:568:GLN:OE1	1:B:571:ARG:NH1	2.37	0.58
1:B:558:GLU:HB3	1:B:576:TYR:CD1	2.38	0.57
1:B:803:VAL:HG12	1:B:806:ARG:HD3	1.85	0.57
1:B:836:PRO:HB3	1:B:837:PRO:C	2.24	0.57
1:B:732:TYR:HB2	1:B:745:GLN:HB3	1.86	0.57
1:B:727:LEU:HB2	1:B:729:LEU:HD21	1.85	0.57
1:A:391:ASP:OD2	1:A:391:ASP:N	2.36	0.57
1:B:722:ARG:HH11	1:B:722:ARG:CG	2.16	0.57
1:A:561:GLU:CD	1:A:561:GLU:H	2.07	0.57
1:A:305:PRO:HA	1:A:308:TYR:CD2	2.40	0.57
1:A:306:PRO:HB3	1:A:876:ASN:OD1	2.05	0.57
1:B:322:ARG:NH2	1:B:334:LYS:HB2	2.13	0.57
1:B:699:HIS:CD2	1:B:699:HIS:H	2.22	0.57
1:B:664:LYS:HG2	1:B:685:VAL:CG2	2.35	0.56
1:A:417:HIS:HD1	1:A:417:HIS:C	2.08	0.56
1:B:417:HIS:CE1	1:B:578:MET:HG3	2.39	0.56
1:B:696:ILE:HB	1:B:744:LEU:HB2	1.88	0.56
1:B:722:ARG:HH11	1:B:722:ARG:CB	2.18	0.56
1:B:300:ILE:CG1	1:B:304:TYR:CE2	2.89	0.56
1:B:715:LEU:O	1:B:719:LEU:HD23	2.06	0.56
1:B:746:TYR:C	1:B:746:TYR:CD2	2.79	0.56
1:B:885:MET:O	1:B:888:ALA:HB2	2.05	0.56
1:A:294:ARG:NH2	1:A:317:LEU:HB2	2.21	0.56
1:A:691:HIS:ND1	2:A:2008:HOH:O	1.98	0.56
1:A:582:MET:O	1:A:586:VAL:HG23	2.05	0.56
1:A:302:TYR:HD1	1:A:331:ALA:HA	1.71	0.56
1:A:751:THR:HG23	1:A:754:GLU:HG3	1.88	0.56
1:A:805:ASP:O	1:A:810:ASN:ND2	2.38	0.56
1:B:751:THR:HG22	1:B:754:GLU:N	2.19	0.56
1:A:360:MET:HG2	1:A:364:ASP:HB2	1.87	0.56
1:B:300:ILE:CA	1:B:304:TYR:CE2	2.81	0.56
1:A:335:PHE:HD2	1:A:335:PHE:O	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:PHE:CD1	1:B:357:TRP:CZ3	2.93	0.55
1:B:830:ARG:HH12	1:B:903:LYS:NZ	2.03	0.55
1:A:313:GLU:OE1	1:A:313:GLU:HA	2.07	0.55
1:B:398:LEU:CD1	1:B:554:TYR:CE2	2.90	0.55
1:B:669:ARG:NH1	1:B:683:THR:CG2	2.70	0.55
1:A:318:VAL:O	1:A:322:ARG:N	2.39	0.55
1:A:354:LEU:HD21	1:A:381:TYR:CD1	2.41	0.55
1:A:919:GLN:HB3	1:B:922:GLN:HE22	1.71	0.55
1:B:400:GLN:HE22	1:B:711:GLN:NE2	2.05	0.55
1:A:669:ARG:NH2	2:A:2006:HOH:O	2.38	0.55
1:B:311:SER:HA	1:B:314:GLU:OE2	2.06	0.55
1:B:806:ARG:N	1:B:806:ARG:HD2	2.23	0.55
1:A:322:ARG:NH2	1:A:338:CYS:HG	2.02	0.54
1:A:354:LEU:HD23	1:A:354:LEU:O	2.07	0.54
1:B:645:ASN:OD1	1:B:645:ASN:C	2.45	0.54
1:B:837:PRO:O	1:B:840:LYS:CE	2.50	0.54
1:B:300:ILE:HG13	1:B:304:TYR:CE2	2.42	0.54
1:B:649:PHE:CE2	1:B:664:LYS:HA	2.42	0.54
1:A:333:THR:HG22	1:A:360:MET:HE2	1.89	0.54
1:A:657:ASP:HB3	1:A:660:ILE:HD12	1.88	0.54
1:A:803:VAL:HG12	1:A:806:ARG:HD3	1.90	0.54
1:A:305:PRO:O	1:A:334:LYS:NZ	2.39	0.54
1:A:942:ARG:HD3	1:B:835:MET:CG	2.38	0.54
1:B:738:SER:CB	1:B:741:HIS:HE1	2.13	0.54
1:A:909:GLN:HG3	1:A:912:LEU:HG	1.89	0.54
1:A:533:LEU:C	1:A:533:LEU:HD23	2.28	0.54
1:A:839:MET:HG2	1:A:925:LEU:HD23	1.90	0.54
1:A:843:LYS:HE2	1:A:847:GLU:OE2	2.06	0.54
1:A:879:LEU:HD11	1:A:905:GLU:HG3	1.90	0.54
1:A:319:TRP:O	1:A:322:ARG:HB2	2.08	0.54
1:A:677:LEU:CD2	1:A:700:GLY:HA3	2.38	0.54
1:A:737:THR:CG2	1:A:741:HIS:CD2	2.90	0.54
1:B:325:LEU:C	1:B:327:SER:H	2.11	0.54
1:B:342:LYS:HB3	1:B:346:GLU:HG3	1.90	0.54
1:B:702:ASP:OD1	1:B:704:ARG:NH2	2.39	0.54
1:B:705:GLN:HG2	1:B:827:ILE:HD13	1.90	0.54
1:B:788:ILE:HG13	1:B:860:PHE:HB2	1.90	0.54
1:B:716:MET:HG2	1:B:878:MET:HE2	1.89	0.53
1:B:639:GLN:HG2	1:B:647:THR:HG21	1.89	0.53
1:B:730:THR:HG22	1:B:818:LYS:HD3	1.90	0.53
1:B:836:PRO:CB	1:B:837:PRO:C	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:GLU:O	1:A:786:THR:HG23	2.08	0.53
1:B:306:PRO:HG2	1:B:879:LEU:CD1	2.39	0.53
1:B:313:GLU:HG2	1:B:314:GLU:HG3	1.90	0.53
1:B:669:ARG:HH11	1:B:683:THR:CB	2.19	0.53
1:B:322:ARG:HD3	1:B:335:PHE:HD1	1.73	0.53
1:B:369:LEU:HD11	1:B:386:LEU:HD11	1.90	0.53
1:B:631:LYS:HD2	1:B:635:LEU:CD2	2.37	0.53
1:A:614:LEU:HD21	1:A:636:LEU:HD23	1.91	0.53
1:A:776:PRO:HB2	1:A:777:TYR:HD1	1.73	0.53
1:B:306:PRO:CG	1:B:879:LEU:HD12	2.38	0.53
1:A:304:TYR:HB2	1:A:305:PRO:HD3	1.90	0.53
1:A:739:SER:O	1:A:740:LYS:CG	2.56	0.53
1:B:654:PHE:CD1	1:B:655:PRO:HD2	2.43	0.53
1:A:323:PHE:HA	1:A:353:MET:HE1	1.90	0.53
1:B:534:CYS:O	1:B:538:ILE:HG13	2.08	0.53
1:B:709:ILE:HD12	1:B:801:LEU:HD13	1.91	0.53
1:B:715:LEU:HD12	1:B:881:LEU:HD12	1.91	0.53
1:B:732:TYR:OH	1:B:822:ILE:O	2.25	0.53
1:A:580:LEU:HB3	1:A:581:LYS:CE	2.39	0.52
1:A:807:HIS:H	1:A:810:ASN:HB2	1.73	0.52
1:B:348:THR:HA	1:B:351:LEU:CD2	2.39	0.52
1:A:782:GLU:O	1:A:786:THR:CG2	2.58	0.52
1:B:311:SER:OG	1:B:314:GLU:HB2	2.08	0.52
1:B:319:TRP:CD1	1:B:323:PHE:CE2	2.97	0.52
1:A:421:PHE:N	1:A:421:PHE:CD1	2.78	0.52
1:B:292:SER:O	1:B:295:ASP:HB3	2.10	0.52
1:A:405:LEU:HD23	1:A:533:LEU:HD21	1.90	0.52
1:B:719:LEU:HD23	1:B:719:LEU:N	2.25	0.52
1:B:806:ARG:CZ	1:B:810:ASN:HD22	2.23	0.52
1:A:410:PRO:O	1:A:414:VAL:HG23	2.10	0.52
1:A:560:GLU:OE2	1:A:739:SER:OG	2.27	0.52
1:A:649:PHE:HE1	1:A:662:ILE:HG13	1.73	0.52
1:B:410:PRO:O	1:B:414:VAL:HG22	2.10	0.52
1:B:551:PHE:O	1:B:555:LEU:HG	2.09	0.52
1:B:669:ARG:NH1	1:B:683:THR:CB	2.73	0.52
1:B:830:ARG:CZ	1:B:903:LYS:HZ2	2.23	0.52
1:A:811:LEU:C	1:A:812:LEU:HD23	2.31	0.51
1:A:854:SER:O	1:A:855:GLU:C	2.48	0.51
1:B:319:TRP:NE1	1:B:323:PHE:CE2	2.78	0.51
1:B:575:MET:HE2	1:B:576:TYR:HA	1.91	0.51
1:A:712:MET:O	1:A:716:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:SER:CA	1:B:314:GLU:HB2	2.38	0.51
1:B:577:ALA:O	1:B:581:LYS:HD2	2.11	0.51
1:B:823:ASP:OD1	1:B:824:PHE:N	2.43	0.51
1:B:839:MET:HG2	1:B:925:LEU:HD23	1.92	0.51
1:B:710:LEU:O	1:B:714:THR:OG1	2.26	0.51
1:B:737:THR:HG23	1:B:742:GLY:HA2	1.91	0.51
1:A:626:ASN:HA	1:A:629:THR:HG23	1.93	0.51
1:B:375:HIS:CD2	1:B:377:GLN:N	2.70	0.51
1:B:733:LYS:H	1:B:745:GLN:NE2	2.06	0.51
1:B:763:HIS:CD2	1:B:848:ALA:HA	2.45	0.51
1:B:827:ILE:CG2	1:B:828:LEU:HG	2.40	0.51
1:A:836:PRO:HB2	1:A:837:PRO:CA	2.41	0.51
1:B:664:LYS:HG3	1:B:685:VAL:HG21	1.89	0.51
1:A:405:LEU:CD2	1:A:533:LEU:CD2	2.88	0.51
1:B:822:ILE:HG23	1:B:823:ASP:N	2.26	0.51
1:A:339:ILE:C	1:A:341:TRP:H	2.11	0.51
1:A:363:GLU:HA	1:A:366:LEU:HD12	1.92	0.50
1:A:737:THR:HB	1:A:741:HIS:HD2	1.74	0.50
1:B:300:ILE:HG13	1:B:304:TYR:HE2	1.76	0.50
1:A:610:GLU:OE2	1:A:613:LYS:HD2	2.11	0.50
1:A:790:SER:CB	1:A:819:LEU:H	2.24	0.50
1:B:403:GLN:HE22	1:B:406:LYS:NZ	2.10	0.50
1:B:417:HIS:O	1:B:420:ILE:HG13	2.12	0.50
1:B:308:TYR:HD1	1:B:310:LEU:HD12	1.77	0.50
1:A:827:ILE:HG22	1:A:892:ASP:HB2	1.93	0.50
1:B:304:TYR:HB2	1:B:305:PRO:HD3	1.94	0.50
1:A:854:SER:C	1:A:856:HIS:N	2.64	0.49
1:A:339:ILE:HD13	1:A:350:ALA:HB1	1.94	0.49
1:B:664:LYS:HG2	1:B:685:VAL:HG23	1.93	0.49
1:B:722:ARG:HH11	1:B:722:ARG:HG3	1.75	0.49
1:A:409:ASP:CB	1:A:412:HIS:NE2	2.64	0.49
1:B:321:PHE:O	1:B:325:LEU:HB2	2.12	0.49
1:A:909:GLN:OE1	1:A:909:GLN:CA	2.60	0.49
1:B:810:ASN:HA	1:B:822:ILE:HG22	1.95	0.49
1:A:412:HIS:CD2	1:A:412:HIS:N	2.77	0.49
1:B:406:LYS:NZ	1:B:887:ASP:O	2.46	0.49
1:A:645:ASN:O	1:A:648:ASN:O	2.30	0.49
1:B:329:LYS:CD	1:B:361:ASP:OD1	2.58	0.49
1:B:302:TYR:CE1	1:B:331:ALA:CB	2.94	0.49
1:B:667:PRO:O	1:B:670:THR:HG22	2.10	0.49
1:B:719:LEU:N	1:B:719:LEU:CD2	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:LYS:HD3	1:B:786:THR:HB	1.94	0.49
1:A:294:ARG:NH1	1:A:298:HIS:CD2	2.81	0.49
1:B:776:PRO:HB2	1:B:777:TYR:CD1	2.36	0.49
1:B:930:THR:HA	1:B:936:LEU:HD12	1.94	0.49
1:B:708:LEU:HD22	1:B:712:MET:HG2	1.94	0.49
1:B:752:VAL:HG23	1:B:811:LEU:O	2.12	0.49
1:A:763:HIS:HD2	1:A:779:ILE:CD1	2.26	0.48
1:B:705:GLN:CG	1:B:827:ILE:HD13	2.42	0.48
1:B:734:VAL:HG13	1:B:744:LEU:HD23	1.95	0.48
1:B:930:THR:HA	1:B:936:LEU:CD1	2.43	0.48
1:B:751:THR:HG22	1:B:754:GLU:HG3	1.95	0.48
1:B:331:ALA:HB1	1:B:357:TRP:CZ2	2.43	0.48
1:B:362:VAL:O	1:B:365:ALA:HB3	2.14	0.48
1:B:769:HIS:ND1	1:B:815:THR:HB	2.29	0.48
1:B:826:TYR:HB3	1:B:830:ARG:O	2.13	0.48
1:B:768:LYS:HB3	1:B:769:HIS:CD2	2.49	0.48
1:B:810:ASN:C	1:B:811:LEU:HD23	2.34	0.48
1:A:551:PHE:CZ	1:A:555:LEU:HD11	2.49	0.48
1:B:379:ARG:HH12	1:B:407:TYR:HB2	1.77	0.48
1:B:339:ILE:HG13	1:B:340:ASN:H	1.79	0.48
1:B:841:LEU:O	1:B:932:VAL:HG21	2.14	0.48
1:A:417:HIS:C	1:A:417:HIS:ND1	2.67	0.48
1:B:812:LEU:H	1:B:812:LEU:CD2	2.26	0.48
1:A:836:PRO:HB2	1:A:837:PRO:HA	1.96	0.48
1:B:300:ILE:CG1	1:B:304:TYR:HE2	2.27	0.48
1:B:339:ILE:HG13	1:B:340:ASN:N	2.29	0.48
1:B:381:TYR:C	1:B:381:TYR:CD2	2.87	0.48
1:B:631:LYS:HD2	1:B:635:LEU:HD21	1.94	0.48
1:B:807:HIS:O	1:B:810:ASN:HB2	2.14	0.48
1:A:852:ILE:HA	1:A:852:ILE:HD12	1.60	0.47
1:B:699:HIS:O	1:B:740:LYS:O	2.32	0.47
1:A:323:PHE:HE1	1:A:349:GLN:OE1	1.96	0.47
1:A:304:TYR:CB	1:A:305:PRO:HD3	2.44	0.47
1:A:306:PRO:HD2	1:A:308:TYR:HD2	1.73	0.47
1:A:323:PHE:HA	1:A:353:MET:CE	2.44	0.47
1:B:636:LEU:HD12	1:B:670:THR:HG21	1.96	0.47
1:A:723:GLU:OE1	1:A:723:GLU:CA	2.63	0.47
1:B:375:HIS:CD2	1:B:376:PRO:HD2	2.50	0.47
1:B:631:LYS:O	1:B:635:LEU:HD23	2.14	0.47
1:A:409:ASP:CB	1:A:412:HIS:HE2	2.27	0.47
1:A:841:LEU:O	1:A:932:VAL:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:HIS:NE2	1:A:861:ARG:HD2	2.30	0.47
1:B:316:ASP:O	1:B:319:TRP:HB3	2.15	0.47
1:B:763:HIS:HE1	1:B:777:TYR:CE2	2.33	0.47
1:B:806:ARG:CZ	1:B:810:ASN:ND2	2.78	0.47
1:A:320:LYS:HD2	1:A:321:PHE:HE2	1.79	0.47
1:A:546:THR:O	1:A:549:ASN:HB3	2.15	0.47
1:A:651:PRO:HA	1:A:662:ILE:O	2.14	0.47
1:A:835:MET:HG3	1:B:943:PHE:HE2	1.80	0.47
1:A:925:LEU:O	1:A:929:ILE:HG13	2.15	0.47
1:B:335:PHE:C	1:B:335:PHE:CD2	2.88	0.47
1:A:305:PRO:HA	1:A:308:TYR:CE2	2.50	0.47
1:B:295:ASP:O	1:B:299:THR:HG23	2.15	0.47
1:A:363:GLU:HB3	1:A:877:VAL:HG13	1.95	0.46
1:A:830:ARG:CZ	1:A:830:ARG:HB3	2.44	0.46
1:B:730:THR:O	1:B:730:THR:OG1	2.30	0.46
1:B:751:THR:HG22	1:B:754:GLU:CG	2.45	0.46
1:B:830:ARG:NH2	1:B:903:LYS:NZ	2.58	0.46
1:B:885:MET:O	1:B:888:ALA:CB	2.62	0.46
1:B:719:LEU:O	1:B:723:GLU:HG2	2.16	0.46
1:B:843:LYS:CA	1:B:932:VAL:CG1	2.92	0.46
1:A:335:PHE:CD1	1:A:357:TRP:CH2	2.87	0.46
1:A:354:LEU:HD23	1:A:354:LEU:C	2.36	0.46
1:A:835:MET:HG3	1:B:943:PHE:CE2	2.50	0.46
1:B:408:GLU:CB	1:B:409:ASP:HA	2.45	0.46
1:B:654:PHE:HD1	1:B:655:PRO:CD	2.27	0.46
1:B:798:THR:CG2	1:B:803:VAL:HB	2.41	0.46
1:B:407:TYR:N	1:B:407:TYR:CD2	2.78	0.46
1:B:634:LYS:HE2	1:B:634:LYS:CA	2.43	0.46
1:A:308:TYR:HB3	1:A:310:LEU:HB2	1.97	0.46
1:A:862:LYS:O	1:A:866:THR:CG2	2.64	0.46
1:B:383:VAL:HA	1:B:386:LEU:HD12	1.97	0.46
1:B:389:ALA:HA	1:B:390:PRO:HD2	1.73	0.46
1:A:312:SER:O	1:A:315:GLN:HG3	2.16	0.46
1:A:610:GLU:OE1	1:A:643:LYS:HB2	2.16	0.46
1:B:326:SER:HA	1:B:357:TRP:CE2	2.51	0.46
1:B:888:ALA:O	1:B:889:THR:CG2	2.59	0.45
1:A:318:VAL:C	1:A:322:ARG:HG3	2.37	0.45
1:A:922:GLN:O	1:A:926:ASP:OD2	2.34	0.45
1:B:547:LEU:HD23	1:B:547:LEU:HA	1.83	0.45
1:B:612:VAL:HG22	1:B:741:HIS:HD2	1.80	0.45
1:A:306:PRO:HD3	1:A:308:TYR:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:MET:HG2	1:B:878:MET:HE1	1.99	0.45
1:B:777:TYR:HB2	1:B:779:ILE:CD1	2.46	0.45
1:B:763:HIS:NE2	1:B:848:ALA:O	2.41	0.45
1:A:869:LEU:HD23	1:A:869:LEU:HA	1.85	0.45
1:A:339:ILE:CG2	1:A:350:ALA:HB2	2.43	0.45
1:A:400:GLN:HG2	1:A:881:LEU:CD2	2.46	0.45
1:B:552:TYR:OH	1:B:605:ARG:NE	2.50	0.45
1:A:732:TYR:OH	1:A:822:ILE:HG12	2.16	0.45
1:A:899:LYS:HB3	1:A:903:LYS:HE2	1.98	0.45
1:A:719:LEU:O	1:A:723:GLU:HG2	2.17	0.45
1:B:587:LEU:HB3	1:B:598:PHE:HB2	1.99	0.45
1:A:314:GLU:CA	1:A:317:LEU:HG	2.46	0.45
1:A:321:PHE:O	1:A:325:LEU:HD23	2.17	0.45
1:A:703:LEU:HD12	1:A:742:GLY:HA3	1.99	0.44
1:B:558:GLU:HB3	1:B:576:TYR:HD1	1.79	0.44
1:B:651:PRO:HA	1:B:662:ILE:O	2.17	0.44
1:A:302:TYR:CD1	1:A:331:ALA:HA	2.50	0.44
1:A:305:PRO:HB3	1:A:308:TYR:HB2	2.00	0.44
1:A:313:GLU:CD	1:A:313:GLU:N	2.70	0.44
1:A:763:HIS:HB3	1:A:767:ARG:NH2	2.32	0.44
1:B:375:HIS:CD2	1:B:376:PRO:CD	3.00	0.44
1:B:544:ASN:OD1	1:B:544:ASN:C	2.56	0.44
1:B:785:ASP:O	1:B:789:LYS:HG3	2.17	0.44
1:A:315:GLN:O	1:A:319:TRP:HB2	2.17	0.44
1:B:330:LYS:HE3	1:B:334:LYS:HE2	1.99	0.44
1:B:360:MET:SD	1:B:364:ASP:HB3	2.58	0.44
1:A:421:PHE:N	1:A:421:PHE:HD1	2.14	0.44
1:B:325:LEU:C	1:B:327:SER:N	2.70	0.44
1:B:678:MET:HA	1:B:679:PRO:HD3	1.82	0.44
1:B:810:ASN:HA	1:B:822:ILE:CG2	2.46	0.44
1:B:830:ARG:NH1	1:B:903:LYS:NZ	2.64	0.44
1:A:573:HIS:C	1:A:573:HIS:HD2	2.17	0.44
1:B:763:HIS:HE2	1:B:848:ALA:C	2.19	0.44
1:B:805:ASP:O	1:B:810:ASN:ND2	2.51	0.44
1:A:328:HIS:O	1:A:331:ALA:HB3	2.18	0.44
1:B:354:LEU:C	1:B:354:LEU:CD2	2.86	0.44
1:B:612:VAL:CG2	1:B:741:HIS:CD2	3.01	0.44
1:B:677:LEU:HD11	1:B:700:GLY:HA3	1.99	0.44
1:B:736:ALA:HA	1:B:742:GLY:HA3	2.00	0.44
1:A:332:LEU:O	1:A:336:LEU:HD23	2.18	0.43
1:B:342:LYS:HD2	1:B:342:LYS:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:MET:CG	1:B:364:ASP:CB	2.93	0.43
1:B:379:ARG:HH12	1:B:407:TYR:CB	2.31	0.43
1:A:313:GLU:OE1	1:A:313:GLU:N	2.51	0.43
1:A:591:ASN:O	1:A:595:ARG:HG3	2.17	0.43
1:A:737:THR:HB	1:A:741:HIS:CD2	2.53	0.43
1:A:837:PRO:O	1:A:840:LYS:HE3	2.18	0.43
1:B:578:MET:O	1:B:582:MET:HG3	2.18	0.43
1:A:319:TRP:HA	1:A:322:ARG:CG	2.47	0.43
1:B:298:HIS:NE2	1:B:321:PHE:HB2	2.33	0.43
1:B:612:VAL:CG2	1:B:741:HIS:HD2	2.31	0.43
1:B:722:ARG:CA	1:B:722:ARG:NH1	2.79	0.43
1:A:734:VAL:CG2	1:A:744:LEU:HD23	2.36	0.43
1:A:807:HIS:O	1:A:810:ASN:HB2	2.18	0.43
1:B:408:GLU:HA	1:B:410:PRO:HD3	1.99	0.43
1:B:631:LYS:CD	1:B:635:LEU:HD23	2.48	0.43
1:A:751:THR:CG2	1:A:754:GLU:CD	2.86	0.43
1:B:322:ARG:NH2	1:B:334:LYS:CB	2.80	0.43
1:B:610:GLU:CD	1:B:643:LYS:HG3	2.39	0.43
1:B:631:LYS:CD	1:B:635:LEU:CD2	2.95	0.43
1:B:558:GLU:CB	1:B:576:TYR:CD1	3.01	0.43
1:B:660:ILE:HD12	1:B:693:TYR:CD2	2.53	0.43
1:A:553:TRP:CZ3	1:A:737:THR:HG23	2.54	0.43
1:A:723:GLU:O	1:A:724:ASN:CB	2.65	0.43
1:A:763:HIS:O	1:A:767:ARG:HB2	2.19	0.43
1:B:331:ALA:HB3	1:B:357:TRP:HE1	1.84	0.43
1:A:827:ILE:HG22	1:A:892:ASP:HB3	2.00	0.43
1:A:798:THR:CG2	1:A:803:VAL:HB	2.44	0.42
1:B:314:GLU:HB3	1:B:317:LEU:HD23	2.01	0.42
1:A:561:GLU:CD	1:A:561:GLU:N	2.71	0.42
1:A:830:ARG:NH1	1:A:892:ASP:OD1	2.53	0.42
1:B:317:LEU:O	1:B:320:LYS:HG2	2.19	0.42
1:A:862:LYS:O	1:A:866:THR:HG23	2.19	0.42
1:B:360:MET:HE1	1:B:365:ALA:HA	2.00	0.42
1:A:703:LEU:HB2	1:A:736:ALA:HB2	2.01	0.42
1:A:933:MET:HA	1:A:934:PRO:HD3	1.75	0.42
1:B:614:LEU:HD12	1:B:614:LEU:C	2.39	0.42
1:B:618:VAL:HG21	1:B:632:PHE:CD2	2.55	0.42
1:A:362:VAL:HG13	1:A:386:LEU:HD23	2.02	0.42
1:A:552:TYR:CG	1:A:601:LEU:HD22	2.55	0.42
1:A:673:PHE:HB2	1:A:679:PRO:HD2	2.01	0.42
1:B:413:ILE:HD13	1:B:575:MET:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ARG:CZ	1:A:298:HIS:NE2	2.83	0.42
1:A:664:LYS:HB2	1:A:685:VAL:HG22	2.00	0.42
1:A:315:GLN:HB3	1:A:338:CYS:HB3	2.01	0.42
1:A:591:ASN:ND2	1:A:591:ASN:N	2.68	0.42
1:A:762:ILE:HD13	1:A:813:LEU:HD21	2.02	0.42
1:B:930:THR:HG22	1:B:936:LEU:HB3	2.02	0.42
1:A:843:LYS:O	1:A:847:GLU:HG3	2.19	0.42
1:B:300:ILE:HA	1:B:304:TYR:CD2	2.49	0.42
1:B:719:LEU:HD12	1:B:874:HIS:CG	2.55	0.42
1:B:843:LYS:HA	1:B:932:VAL:HG11	2.01	0.42
1:A:299:THR:O	1:A:303:ARG:HB2	2.19	0.42
1:B:375:HIS:CD2	1:B:376:PRO:N	2.88	0.42
1:B:763:HIS:O	1:B:767:ARG:HB2	2.20	0.42
1:A:298:HIS:HB3	1:A:302:TYR:CE2	2.55	0.41
1:A:580:LEU:HD23	1:A:580:LEU:HA	1.86	0.41
1:A:871:LEU:HD23	1:A:871:LEU:HA	1.92	0.41
1:B:395:LEU:HD21	1:B:550:TYR:CD2	2.55	0.41
1:B:746:TYR:CE2	1:B:748:ASP:HA	2.55	0.41
1:A:648:ASN:OD1	1:A:664:LYS:HE2	2.19	0.41
1:A:843:LYS:HA	1:A:932:VAL:HG13	2.03	0.41
1:B:305:PRO:HA	1:B:306:PRO:HD3	1.80	0.41
1:B:746:TYR:HE2	1:B:748:ASP:HA	1.85	0.41
1:A:570:GLU:O	1:A:574:ASP:OD1	2.39	0.41
1:A:677:LEU:HD22	1:A:700:GLY:CA	2.48	0.41
1:A:733:LYS:H	1:A:745:GLN:HB2	1.85	0.41
1:A:835:MET:HG3	1:A:836:PRO:HD2	2.02	0.41
1:B:598:PHE:CD2	1:B:598:PHE:C	2.94	0.41
1:A:320:LYS:HD2	1:A:321:PHE:CE2	2.56	0.41
1:A:339:ILE:C	1:A:341:TRP:N	2.73	0.41
1:A:400:GLN:HE21	1:A:885:MET:CG	2.33	0.41
1:A:638:GLU:HG2	1:A:641:MET:HB2	2.03	0.41
1:B:552:TYR:CD2	1:B:601:LEU:HD22	2.56	0.41
1:B:634:LYS:HA	1:B:634:LYS:CE	2.37	0.41
1:B:716:MET:CG	1:B:878:MET:HE2	2.49	0.41
1:B:375:HIS:HD2	1:B:376:PRO:N	2.18	0.41
1:B:915:GLU:O	1:B:919:GLN:HG3	2.21	0.41
1:A:375:HIS:CD2	1:A:377:GLN:H	2.39	0.41
1:A:662:ILE:H	1:A:662:ILE:HG12	1.79	0.41
1:A:709:ILE:HD13	1:A:709:ILE:HA	1.90	0.41
1:B:621:GLU:HA	1:B:622:PRO:HD3	1.90	0.41
1:B:629:THR:CG2	1:B:672:LEU:HD12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:THR:HG1	1:A:373:PHE:HE2	1.63	0.41
1:A:405:LEU:CD2	1:A:533:LEU:HD21	2.51	0.41
1:A:533:LEU:HD23	1:A:534:CYS:N	2.36	0.41
1:B:300:ILE:CA	1:B:304:TYR:HE2	2.15	0.41
1:B:332:LEU:HD13	1:B:357:TRP:CG	2.55	0.41
1:A:634:LYS:HA	1:A:634:LYS:HD2	1.84	0.41
1:B:783:VAL:HA	1:B:786:THR:HG23	2.03	0.40
1:B:804:GLY:O	1:B:805:ASP:HB3	2.21	0.40
1:B:556:SER:HB2	1:B:605:ARG:HH21	1.85	0.40
1:B:686:THR:OG1	1:B:691:HIS:HB2	2.21	0.40
1:B:631:LYS:HD3	1:B:635:LEU:HD23	2.03	0.40
1:A:782:GLU:CD	1:A:782:GLU:H	2.23	0.40
1:A:350:ALA:O	1:A:353:MET:HB2	2.22	0.40
1:A:699:HIS:O	1:A:699:HIS:CD2	2.74	0.40
1:B:806:ARG:HA	1:B:810:ASN:HD22	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:TYR:OH	1:A:782:GLU:OE1[6_555]	2.12	0.08

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	537/696 (77%)	508 (95%)	23 (4%)	6 (1%)	14 42
1	B	537/696 (77%)	512 (95%)	21 (4%)	4 (1%)	22 54
All	All	1074/1392 (77%)	1020 (95%)	44 (4%)	10 (1%)	17 48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	PRO
1	A	737	THR
1	B	836	PRO
1	A	304	TYR
1	B	305	PRO
1	A	836	PRO
1	B	306	PRO
1	B	408	GLU
1	A	362	VAL
1	A	776	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/612 (80%)	399 (82%)	90 (18%)	1	5
1	B	488/612 (80%)	416 (85%)	72 (15%)	3	9
All	All	977/1224 (80%)	815 (83%)	162 (17%)	2	7

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	ILE
1	A	297	LEU
1	A	303	ARG
1	A	309	VAL
1	A	313	GLU
1	A	317	LEU
1	A	333	THR
1	A	335	PHE
1	A	349	GLN
1	A	351	LEU
1	A	363	GLU
1	A	370	SER
1	A	373	PHE
1	A	378	VAL

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Mol	Chain	Res	Type
1	A	391	ASP
1	A	393	ASP
1	A	396	LEU
1	A	412	HIS
1	A	416	LEU
1	A	417	HIS
1	A	421	PHE
1	A	532	ASN
1	A	534	CYS
1	A	540	ARG
1	A	544	ASN
1	A	546	THR
1	A	549	ASN
1	A	561	GLU
1	A	573	HIS
1	A	580	LEU
1	A	581	LYS
1	A	591	ASN
1	A	592	PHE
1	A	594	LEU
1	A	602	ARG
1	A	606	ARG
1	A	611	LEU
1	A	614	LEU
1	A	629	THR
1	A	632	PHE
1	A	634	LYS
1	A	659	GLU
1	A	669	ARG
1	A	671	SER
1	A	674	LYS
1	A	685	VAL
1	A	686	THR
1	A	691	HIS
1	A	708	LEU
1	A	710	LEU
1	A	711	GLN
1	A	715	LEU
1	A	723	GLU
1	A	724	ASN
1	A	725	LEU
1	A	730	THR

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Mol	Chain	Res	Type
1	A	747	VAL
1	A	748	ASP
1	A	750	CYS
1	A	751	THR
1	A	759	GLU
1	A	786	THR
1	A	788	ILE
1	A	791	CYS
1	A	795	CYS
1	A	806	ARG
1	A	807	HIS
1	A	808	LEU
1	A	811	LEU
1	A	812	LEU
1	A	813	LEU
1	A	822	ILE
1	A	827	ILE
1	A	831	ASP
1	A	835	MET
1	A	839	MET
1	A	842	SER
1	A	852	ILE
1	A	854	SER
1	A	866	THR
1	A	889	THR
1	A	896	GLU
1	A	909	GLN
1	A	913	THR
1	A	926	ASP
1	A	927	VAL
1	A	930	THR
1	A	932	VAL
1	A	942	ARG
1	A	948	ARG
1	B	298	HIS
1	B	299	THR
1	B	313	GLU
1	B	314	GLU
1	B	316	ASP
1	B	317	LEU
1	B	321	PHE
1	B	333	THR

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Mol	Chain	Res	Type
1	B	338	CYS
1	B	343	LEU
1	B	348	THR
1	B	351	LEU
1	B	361	ASP
1	B	372	THR
1	B	374	THR
1	B	398	LEU
1	B	399	LEU
1	B	414	VAL
1	B	549	ASN
1	B	571	ARG
1	B	575	MET
1	B	580	LEU
1	B	581	LYS
1	B	592	PHE
1	B	605	ARG
1	B	611	LEU
1	B	614	LEU
1	B	634	LYS
1	B	638	GLU
1	B	645	ASN
1	B	654	PHE
1	B	656	LEU
1	B	670	THR
1	B	677	LEU
1	B	682	LEU
1	B	685	VAL
1	B	702	ASP
1	B	706	ASP
1	B	708	LEU
1	B	710	LEU
1	B	715	LEU
1	B	719	LEU
1	B	722	ARG
1	B	724	ASN
1	B	725	LEU
1	B	730	THR
1	B	741	HIS
1	B	746	TYR
1	B	747	VAL
1	B	750	CYS

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Mol	Chain	Res	Type
1	B	751	THR
1	B	758	ARG
1	B	759	GLU
1	B	782	GLU
1	B	786	THR
1	B	788	ILE
1	B	806	ARG
1	B	811	LEU
1	B	812	LEU
1	B	813	LEU
1	B	819	LEU
1	B	822	ILE
1	B	827	ILE
1	B	839	MET
1	B	842	SER
1	B	876	ASN
1	B	889	THR
1	B	898	ASP
1	B	914	ASP
1	B	923	SER
1	B	927	VAL
1	B	948	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	A	356	ASN
1	A	403	GLN
1	A	412	HIS
1	A	573	HIS
1	A	591	ASN
1	A	639	GLN
1	A	645	ASN
1	A	699	HIS
1	A	711	GLN
1	A	724	ASN
1	A	741	HIS
1	A	763	HIS
1	A	870	HIS
1	A	922	GLN
1	A	939	GLN

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Mol	Chain	Res	Type
1	A	945	GLN
1	B	349	GLN
1	B	375	HIS
1	B	403	GLN
1	B	549	ASN
1	B	573	HIS
1	B	633	GLN
1	B	639	GLN
1	B	691	HIS
1	B	711	GLN
1	B	724	ASN
1	B	741	HIS
1	B	745	GLN
1	B	807	HIS
1	B	810	ASN
1	B	821	HIS
1	B	876	ASN
1	B	919	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	543/696 (78%)	0.35	22 (4%) 37 32	20, 33, 61, 86	0
1	B	543/696 (78%)	0.51	28 (5%) 27 23	22, 40, 74, 87	0
All	All	1086/1392 (78%)	0.43	50 (4%) 32 29	20, 36, 70, 87	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	HIS	9.6
1	A	302	TYR	8.1
1	A	341	TRP	7.3
1	B	322	ARG	7.3
1	B	324	TYR	6.4
1	B	302	TYR	5.9
1	B	341	TRP	5.1
1	A	294	ARG	5.0
1	B	676	ALA	4.8
1	A	322	ARG	4.7
1	B	690	HIS	4.7
1	A	323	PHE	4.3
1	B	636	LEU	4.0
1	B	294	ARG	3.8
1	B	323	PHE	3.7
1	B	293	ILE	3.5
1	B	343	LEU	3.4
1	B	578	MET	3.2
1	A	339	ILE	3.2
1	A	298	HIS	3.1
1	B	682	LEU	3.1
1	A	344	GLU	3.0
1	A	328	HIS	2.9
1	A	324	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	311	SER	2.8
1	B	308	TYR	2.6
1	A	292	SER	2.6
1	A	311	SER	2.5
1	B	684	PHE	2.5
1	B	637	ALA	2.5
1	B	352	TRP	2.5
1	B	339	ILE	2.4
1	A	342	LYS	2.4
1	B	673	PHE	2.4
1	A	352	TRP	2.4
1	A	335	PHE	2.4
1	B	373	PHE	2.3
1	A	308	TYR	2.3
1	B	629	THR	2.3
1	B	333	THR	2.3
1	B	630	GLU	2.2
1	A	330	LYS	2.1
1	A	345	ASP	2.1
1	A	347	VAL	2.1
1	B	347	VAL	2.1
1	A	351	LEU	2.1
1	A	306	PRO	2.0
1	B	378	VAL	2.0
1	B	328	HIS	2.0
1	A	343	LEU	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.