



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:04 PM UTC

PDB ID : 2X6I / pdb_00002x6i
Title : THE CRYSTAL STRUCTURE OF THE DROSOPHILA CLASS III PI3-KINASE VPS34 IN COMPLEX WITH PIK-90
Authors : Miller, S.; Tavshanjian, B.; Oleksy, A.; Perisic, O.; Houseman, B.T.; Shokat, K.M.; Williams, R.L.
Deposited on : 2010-02-17
Resolution : 3.40 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

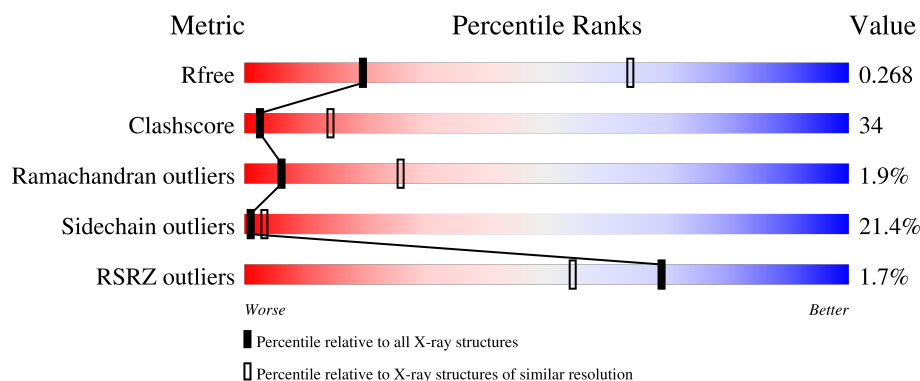
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	 2% 31% 32% 13% 22%
1	B	696	 0% 36% 31% 11% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	090	B	1950	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8976 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.

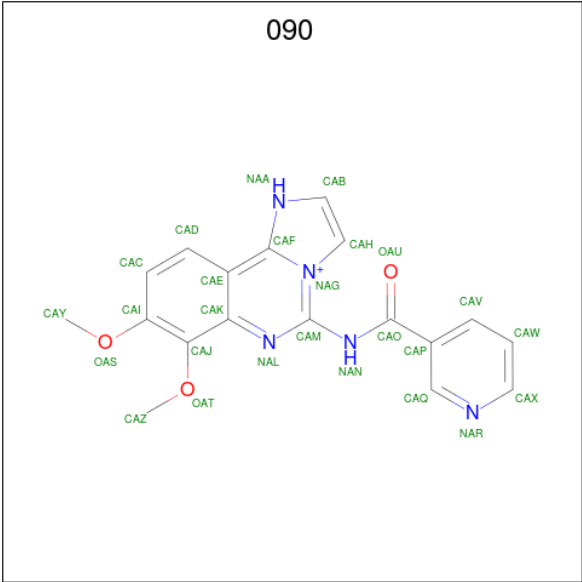
- Molecule 1 is a protein called PHOSPHOTIDYLINOSITOL 3 KINASE 59F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4468	2888	761	792	27			
1	B	544	Total	C	N	O	S	0	0	0
			4456	2881	760	788	27			

There are 10 discrepancies between the modelled and reference sequences:

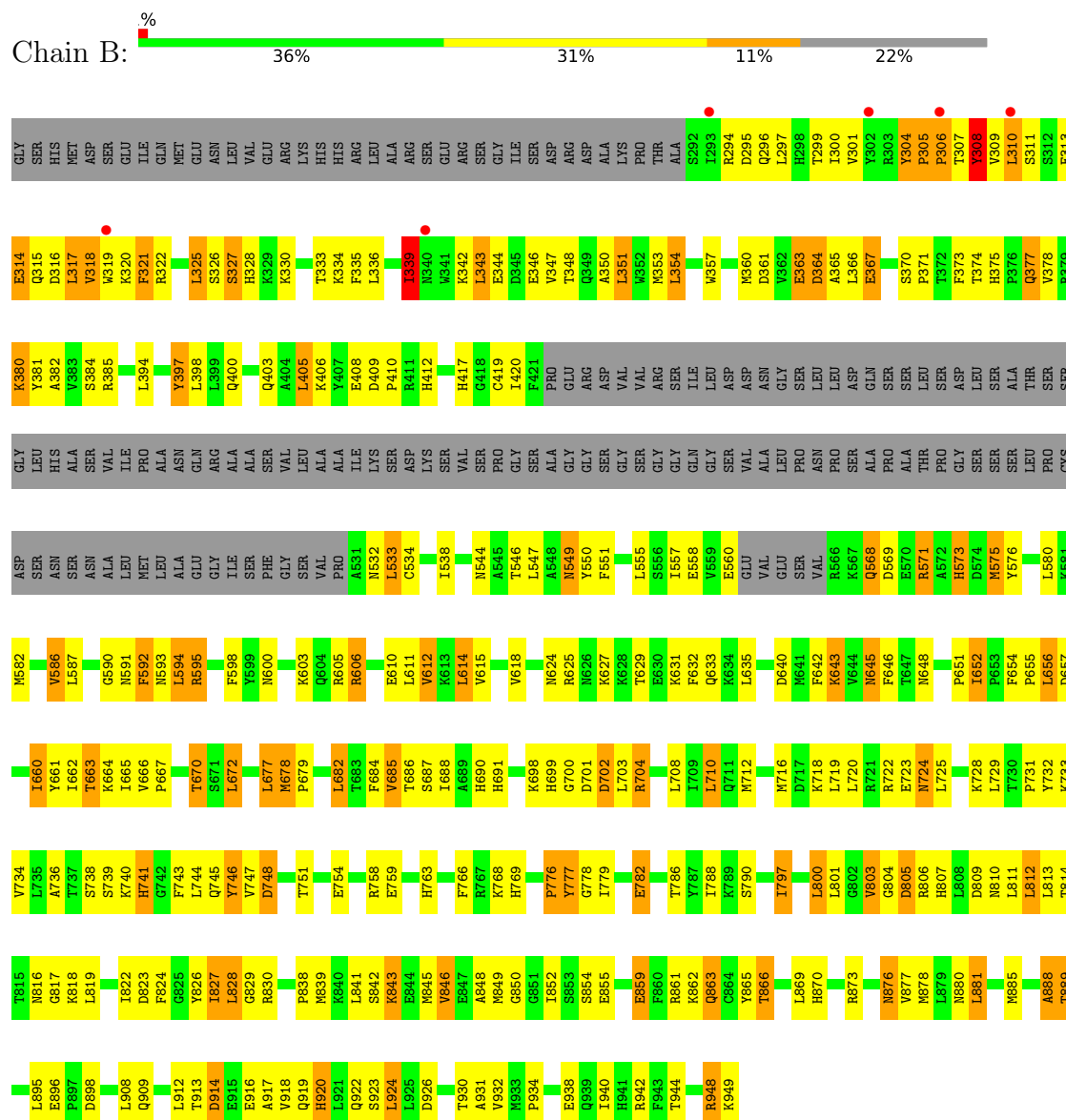
Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	expression tag	UNP Q9W1M7
A	255	SER	-	expression tag	UNP Q9W1M7
A	256	HIS	-	expression tag	UNP Q9W1M7
A	257	MET	-	expression tag	UNP Q9W1M7
A	455	ALA	GLY	engineered mutation	UNP Q9W1M7
B	254	GLY	-	expression tag	UNP Q9W1M7
B	255	SER	-	expression 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 N-(2,3-DIHYDRO-7,8-DIMETHOXYIMIDAZO[1,2-C] QUINAZOLIN-5-YL) NICOTINAMIDE (CCD ID: 090) (formula: C₁₈H₁₆N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	18	5	3		
2	B	1	Total	C	N	O	0	0
			26	18	5	3		

● Molecule 1: PHOSPHOTIDYLINOSITOL 3 KINASE 59F



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.47Å 156.22Å 244.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.83 – 3.40 72.83 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.83-3.40) 97.6 (72.83-3.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.217 , 0.279 0.211 , 0.268	Depositor DCC
R_{free} test set	1426 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	96.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8976	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
090

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	0.92	2/4577 (0.0%)	1.52	97/6197 (1.6%)
1	B	0.75	1/4564 (0.0%)	1.09	9/6177 (0.1%)
All	All	0.84	3/9141 (0.0%)	1.32	106/12374 (0.9%)

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	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	SER	CB-OG	11.78	1.65	1.42
1	B	348	THR	CB-OG1	5.64	1.52	1.43
1	A	592	PHE	CA-C	-5.15	1.45	1.52

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	THR	N-CA-C	-11.27	99.08	111.36
1	A	927	VAL	N-CA-C	-10.26	100.36	110.72
1	A	592	PHE	N-CA-C	-9.81	101.81	113.88
1	A	818	LYS	N-CA-C	-9.52	96.40	110.48
1	A	854	SER	N-CA-C	-9.18	95.00	109.50
1	A	817	GLY	N-CA-C	9.00	125.19	114.48
1	A	852	ILE	N-CA-C	8.65	118.69	110.30
1	A	816	ASN	CA-C-N	-8.55	113.50	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	816	ASN	C-N-CA	-8.55	113.50	123.08
1	A	855	GLU	N-CA-C	-8.44	100.95	111.75
1	A	836	PRO	CA-C-N	7.59	125.13	119.66
1	A	836	PRO	C-N-CA	7.59	125.13	119.66
1	A	663	THR	N-CA-C	7.49	120.03	108.12
1	A	717	ASP	N-CA-C	-7.31	103.39	111.36
1	A	364	ASP	N-CA-C	-6.99	103.42	112.23
1	A	595	ARG	N-CA-C	-6.82	103.84	111.28
1	A	577	ALA	N-CA-C	-6.77	103.92	111.71
1	A	693	TYR	CA-C-N	-6.71	111.54	122.81
1	A	693	TYR	C-N-CA	-6.71	111.54	122.81
1	A	757	ALA	N-CA-C	-6.65	104.11	111.36
1	A	790	SER	N-CA-C	-6.64	104.12	111.82
1	A	786	THR	N-CA-C	-6.64	104.12	111.82
1	A	685	VAL	N-CA-C	-6.59	102.87	110.05
1	A	340	ASN	N-CA-C	6.56	118.98	111.11
1	A	767	ARG	N-CA-C	-6.50	104.28	111.82
1	A	593	ASN	N-CA-C	-6.43	103.78	111.69
1	A	402	VAL	N-CA-C	-6.41	104.25	110.72
1	B	339	ILE	N-CA-C	6.34	117.12	110.72
1	A	915	GLU	N-CA-C	-6.33	104.46	111.36
1	A	888	ALA	N-CA-C	6.32	119.16	111.82
1	A	641	MET	N-CA-C	-6.29	105.10	112.89
1	A	735	LEU	CA-C-N	-6.29	113.28	122.65
1	A	735	LEU	C-N-CA	-6.29	113.28	122.65
1	B	896	GLU	CA-C-N	6.23	125.72	119.24
1	B	896	GLU	C-N-CA	6.23	125.72	119.24
1	A	917	ALA	N-CA-C	-6.12	104.16	111.69
1	A	922	GLN	N-CA-C	-6.11	104.62	111.28
1	A	681	LYS	N-CA-C	-6.05	100.70	110.32
1	A	812	LEU	N-CA-C	6.04	118.88	109.52
1	A	594	LEU	N-CA-C	-6.01	104.29	111.69
1	A	401	LEU	N-CA-C	-6.00	104.86	111.82
1	A	930	THR	N-CA-C	-6.00	104.86	111.82
1	B	678	MET	N-CA-C	5.97	119.13	109.15
1	A	551	PHE	N-CA-C	-5.96	104.78	111.28
1	A	548	ALA	N-CA-C	-5.96	104.78	111.28
1	A	313	GLU	N-CA-C	-5.95	104.74	112.23
1	A	868	TYR	N-CA-C	-5.87	104.96	111.36
1	A	775	GLY	C-N-CD	5.75	133.24	120.60
1	A	596	GLY	N-CA-C	-5.72	105.45	112.77
1	A	867	ALA	N-CA-C	-5.70	105.21	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	LEU	N-CA-C	5.67	117.15	110.97
1	A	636	LEU	N-CA-C	-5.66	105.25	111.82
1	A	817	GLY	CA-C-N	-5.66	112.00	121.39
1	A	817	GLY	C-N-CA	-5.66	112.00	121.39
1	A	369	LEU	N-CA-C	-5.65	106.39	113.28
1	A	321	PHE	N-CA-C	-5.62	106.27	113.23
1	A	784	MET	N-CA-C	-5.60	105.18	111.28
1	A	941	HIS	N-CA-C	-5.60	105.26	111.36
1	A	606	ARG	N-CA-C	-5.57	105.21	112.23
1	A	557	ILE	N-CA-C	-5.54	104.16	111.09
1	A	293	ILE	N-CA-C	-5.53	104.18	111.09
1	A	297	LEU	N-CA-C	-5.51	105.43	111.82
1	A	901	VAL	N-CA-C	-5.50	105.75	111.58
1	A	604	GLN	N-CA-C	-5.50	105.37	111.36
1	A	352	TRP	N-CA-C	-5.49	105.45	111.82
1	A	573	HIS	N-CA-C	-5.43	105.36	111.28
1	A	335	PHE	N-CA-C	-5.39	105.48	111.36
1	A	766	PHE	N-CA-C	-5.38	105.50	111.36
1	A	727	LEU	CA-C-N	-5.38	114.25	122.21
1	A	727	LEU	C-N-CA	-5.38	114.25	122.21
1	A	587	LEU	N-CA-C	-5.37	104.98	112.45
1	A	413	ILE	N-CA-C	-5.36	105.89	111.58
1	A	918	VAL	N-CA-C	-5.34	105.17	110.62
1	A	754	GLU	N-CA-C	-5.32	105.48	111.28
1	B	888	ALA	N-CA-C	5.31	118.22	111.69
1	A	792	ALA	N-CA-C	-5.29	105.51	111.28
1	A	801	LEU	N-CA-C	-5.28	106.52	113.17
1	A	872	ARG	N-CA-C	-5.25	105.67	111.71
1	A	349	GLN	N-CA-C	-5.25	106.03	112.90
1	A	541	ALA	N-CA-C	-5.22	105.70	111.71
1	A	720	LEU	N-CA-C	-5.22	105.65	112.23
1	A	321	PHE	CA-C-N	5.21	127.52	120.38
1	A	321	PHE	C-N-CA	5.21	127.52	120.38
1	A	631	LYS	N-CA-C	-5.16	105.83	111.82
1	A	944	THR	N-CA-C	-5.16	105.78	111.71
1	A	710	LEU	CA-CB-CG	-5.15	98.28	116.30
1	A	936	LEU	N-CA-C	-5.14	105.75	112.23
1	B	569	ASP	N-CA-C	-5.13	106.87	113.23
1	A	837	PRO	O-C-N	5.11	123.55	121.15
1	A	683	THR	CA-C-N	-5.11	114.23	122.81
1	A	683	THR	C-N-CA	-5.11	114.23	122.81
1	B	308	TYR	N-CA-C	5.10	117.75	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	LEU	N-CA-C	-5.08	105.44	111.69
1	A	381	TYR	N-CA-C	-5.08	105.82	111.36
1	B	710	LEU	CA-CB-CG	-5.08	98.54	116.30
1	A	693	TYR	N-CA-C	-5.07	101.37	109.23
1	A	613	LYS	N-CA-C	-5.07	105.65	111.07
1	A	375	HIS	CA-C-N	5.06	126.16	119.84
1	A	375	HIS	C-N-CA	5.06	126.16	119.84
1	A	304	TYR	CA-C-N	-5.05	115.18	120.38
1	A	304	TYR	C-N-CA	-5.05	115.18	120.38
1	A	661	TYR	CA-C-N	-5.03	115.36	122.34
1	A	661	TYR	C-N-CA	-5.03	115.36	122.34
1	A	821	HIS	N-CA-C	5.01	117.74	110.17
1	A	681	LYS	CA-C-O	-5.01	115.35	121.36
1	A	617	LEU	N-CA-C	-5.00	105.93	112.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	591	ASN	Mainchain
1	A	663	THR	Mainchain
1	A	680	ALA	Peptide

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	4468	0	4503	329	0
1	B	4456	0	4498	297	0
2	A	26	0	16	3	0
2	B	26	0	16	10	0
All	All	8976	0	9033	618	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 34.

All (618) 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:292:SER:CB	1:A:292:SER:OG	1.65	1.42
1:B:595:ARG:HG2	1:B:595:ARG:HH11	1.09	1.12
1:B:311:SER:HB2	1:B:314:GLU:HG3	1.24	1.11
1:A:677:LEU:HD11	1:A:700:GLY:H	1.18	1.05
1:B:311:SER:HB2	1:B:314:GLU:CG	1.87	1.05
1:A:677:LEU:HD11	1:A:700:GLY:N	1.72	1.04
1:A:367:GLU:O	1:A:370:SER:HB3	1.56	1.03
1:B:319:TRP:HA	1:B:322:ARG:HE	1.19	1.02
1:A:542:CYS:HB3	1:A:594:LEU:HD21	1.39	1.02
1:A:861:ARG:NH2	1:A:926:ASP:OD2	1.95	1.00
1:B:314:GLU:HA	1:B:317:LEU:HG	1.42	0.99
1:B:408:GLU:HB3	1:B:409:ASP:HA	1.45	0.99
1:A:814:THR:HG23	1:A:818:LYS:H	1.30	0.97
1:A:835:MET:CE	1:B:942:ARG:HD3	1.95	0.97
1:A:808:LEU:H	1:A:808:LEU:HD22	1.30	0.97
1:A:798:THR:HG23	1:A:803:VAL:HB	1.47	0.96
1:B:629:THR:HG22	1:B:672:LEU:HB2	1.46	0.95
1:A:614:LEU:HD21	1:A:636:LEU:HD23	1.51	0.93
1:A:542:CYS:HB3	1:A:594:LEU:CD2	1.98	0.92
1:B:704:ARG:NH1	1:B:889:THR:HG21	1.84	0.91
1:A:308:TYR:HD1	1:A:310:LEU:HD22	1.36	0.90
1:B:405:LEU:HD21	1:B:575:MET:HE1	1.54	0.89
1:A:412:HIS:HB3	1:A:532:ASN:ND2	1.87	0.89
1:A:645:ASN:C	1:A:645:ASN:HD22	1.80	0.89
1:A:835:MET:HE1	1:B:942:ARG:HD3	1.54	0.87
1:B:595:ARG:HG2	1:B:595:ARG:NH1	1.88	0.87
1:A:854:SER:HB2	1:A:857:HIS:H	1.39	0.87
1:B:318:VAL:HG13	1:B:322:ARG:HH22	1.40	0.87
1:B:777:TYR:O	1:B:779:ILE:HG13	1.75	0.86
1:A:756:LEU:HD11	1:A:844:GLU:HG2	1.56	0.86
1:A:776:PRO:HG2	1:A:777:TYR:HD1	1.41	0.86
1:A:335:PHE:HD1	1:A:357:TRP:CZ3	1.94	0.85
1:B:335:PHE:HD2	1:B:336:LEU:HD12	1.39	0.85
1:B:813:LEU:HD12	1:B:818:LYS:O	1.76	0.85
1:B:865:TYR:CD1	1:B:918:VAL:HG13	2.11	0.85
1:A:846:VAL:HG11	1:A:933:MET:HE2	1.59	0.84
1:B:948:ARG:O	1:B:949:LYS:HB2	1.76	0.84
1:B:733:LYS:H	1:B:745:GLN:HE21	1.25	0.84
1:B:534:CYS:O	1:B:538:ILE:HD12	1.78	0.83
1:B:319:TRP:HA	1:B:322:ARG:NE	1.93	0.83
1:B:318:VAL:HG13	1:B:322:ARG:NH2	1.94	0.82
1:A:871:LEU:HD22	1:A:878:MET:HE1	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LEU:HD12	1:A:554:TYR:CE1	2.14	0.82
1:B:682:LEU:H	1:B:682:LEU:HD22	1.46	0.80
1:A:677:LEU:O	1:A:679:PRO:HD3	1.82	0.80
1:A:610:GLU:OE1	1:A:643:LYS:HB2	1.82	0.79
1:A:814:THR:CG2	1:A:818:LYS:H	1.96	0.79
1:B:734:VAL:HG22	1:B:744:LEU:HD22	1.64	0.79
1:B:347:VAL:O	1:B:351:LEU:CD2	2.31	0.78
1:A:608:ILE:O	1:A:612:VAL:HG23	1.83	0.78
1:A:806:ARG:HA	1:A:810:ASN:HD22	1.47	0.78
1:B:347:VAL:O	1:B:351:LEU:HD22	1.83	0.78
1:B:934:PRO:O	1:B:938:GLU:HG3	1.84	0.78
1:B:360:MET:HE3	1:B:361:ASP:H	1.49	0.78
1:A:819:LEU:HD23	1:A:819:LEU:C	2.10	0.77
1:B:412:HIS:HB3	1:B:532:ASN:HD21	1.49	0.77
1:B:682:LEU:HD23	1:B:684:PHE:HE2	1.47	0.77
1:A:727:LEU:HB2	1:A:729:LEU:HD21	1.65	0.77
1:A:303:ARG:O	1:A:304:TYR:HD2	1.67	0.76
1:A:846:VAL:CG1	1:A:933:MET:CE	2.63	0.76
1:A:727:LEU:HD23	1:A:727:LEU:N	2.01	0.76
1:A:602:ARG:CZ	1:A:606:ARG:HD2	2.14	0.76
1:A:913:THR:HG22	1:A:916:GLU:CD	2.11	0.76
1:B:822:ILE:HD11	2:B:1950:090:CAM	2.16	0.76
1:A:751:THR:HG23	1:A:754:GLU:CD	2.10	0.75
1:B:912:LEU:HB3	1:B:916:GLU:HB2	1.67	0.75
1:A:835:MET:HE1	1:B:942:ARG:CD	2.17	0.75
1:B:777:TYR:HD1	1:B:777:TYR:N	1.84	0.75
1:B:948:ARG:HG2	1:B:948:ARG:HH11	1.50	0.75
1:B:335:PHE:CD2	1:B:336:LEU:HD12	2.21	0.75
1:B:595:ARG:H	1:B:595:ARG:HD3	1.51	0.75
1:B:841:LEU:HD23	1:B:845:MET:HE2	1.68	0.75
1:B:827:ILE:CG2	1:B:828:LEU:HG	2.17	0.74
1:A:846:VAL:HG11	1:A:933:MET:CE	2.17	0.74
1:B:360:MET:HE2	1:B:364:ASP:HB3	1.70	0.74
1:A:578:MET:O	1:A:582:MET:HE3	1.88	0.74
1:A:785:ASP:OD1	1:A:789:LYS:HE3	1.88	0.74
1:A:416:LEU:HD12	1:A:535:THR:HG22	1.69	0.74
1:A:814:THR:HG23	1:A:818:LYS:N	2.03	0.74
1:B:300:ILE:O	1:B:305:PRO:HD2	1.87	0.74
1:A:919:GLN:HB3	1:B:922:GLN:HE22	1.52	0.74
1:A:308:TYR:CD1	1:A:310:LEU:HD22	2.23	0.74
1:A:577:ALA:O	1:A:581:LYS:HD2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:VAL:HG12	1:A:806:ARG:HD3	1.68	0.74
1:A:808:LEU:H	1:A:808:LEU:CD2	2.00	0.73
1:B:677:LEU:HD11	1:B:700:GLY:HA3	1.70	0.73
1:B:822:ILE:HD11	2:B:1950:090:NAL	2.03	0.73
1:B:739:SER:O	1:B:740:LYS:HG2	1.88	0.73
1:B:663:THR:OG1	1:B:664:LYS:HG2	1.89	0.73
1:A:645:ASN:C	1:A:645:ASN:ND2	2.46	0.73
1:A:550:TYR:O	1:A:554:TYR:CD2	2.41	0.73
1:A:550:TYR:O	1:A:554:TYR:HD2	1.71	0.73
1:A:708:LEU:HD23	1:A:708:LEU:C	2.14	0.73
1:A:363:GLU:HA	1:A:366:LEU:CD1	2.18	0.72
1:A:808:LEU:HD22	1:A:808:LEU:N	2.04	0.72
1:B:319:TRP:CA	1:B:322:ARG:HE	1.98	0.72
1:A:715:LEU:C	1:A:715:LEU:HD23	2.15	0.72
1:B:822:ILE:HD11	2:B:1950:090:CAO	2.20	0.72
1:A:751:THR:HG23	1:A:754:GLU:CG	2.20	0.72
1:A:645:ASN:HD22	1:A:646:PHE:N	1.88	0.71
1:A:303:ARG:O	1:A:304:TYR:CD2	2.42	0.71
1:A:335:PHE:CD1	1:A:357:TRP:CZ3	2.78	0.71
1:B:777:TYR:N	1:B:777:TYR:CD1	2.57	0.71
1:A:677:LEU:CD1	1:A:700:GLY:H	1.99	0.71
1:B:304:TYR:HB2	1:B:305:PRO:CD	2.20	0.70
1:A:625:ARG:O	1:A:629:THR:HG22	1.91	0.70
1:A:674:LYS:H	1:A:674:LYS:HD3	1.57	0.70
1:B:405:LEU:HD21	1:B:575:MET:CE	2.22	0.70
1:A:739:SER:O	1:A:740:LYS:HG2	1.91	0.69
1:B:412:HIS:HB3	1:B:532:ASN:ND2	2.06	0.69
1:A:737:THR:HG22	1:A:738:SER:N	2.07	0.69
1:B:311:SER:HB2	1:B:314:GLU:CB	2.22	0.68
1:A:743:PHE:C	1:A:744:LEU:HD23	2.19	0.67
1:B:656:LEU:C	1:B:656:LEU:HD23	2.20	0.67
1:A:846:VAL:CG1	1:A:933:MET:HE2	2.25	0.67
1:B:827:ILE:HG22	1:B:828:LEU:HG	1.77	0.67
1:A:811:LEU:N	1:A:811:LEU:HD23	2.09	0.67
1:A:634:LYS:HE2	1:A:634:LYS:O	1.95	0.67
1:A:362:VAL:HG21	1:A:389:ALA:HB2	1.76	0.67
1:A:638:GLU:HG2	1:A:641:MET:HB2	1.77	0.67
1:A:591:ASN:O	1:A:595:ARG:CZ	2.42	0.66
1:A:560:GLU:OE1	1:A:738:SER:HB2	1.96	0.66
1:B:800:LEU:HD13	1:B:908:LEU:HD21	1.76	0.66
1:A:677:LEU:HD22	1:A:678:MET:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:LYS:NZ	2:B:1950:090:HAW	2.10	0.66
1:B:803:VAL:CG1	1:B:806:ARG:HD3	2.26	0.66
1:A:375:HIS:CD2	1:A:377:GLN:HB3	2.31	0.66
1:A:807:HIS:O	1:A:810:ASN:HB2	1.96	0.65
1:A:827:ILE:CG2	1:A:828:LEU:HG	2.26	0.65
1:A:922:GLN:HE22	1:B:919:GLN:HB3	1.62	0.65
1:A:625:ARG:HH21	1:A:674:LYS:HA	1.62	0.65
1:A:677:LEU:HD22	1:A:678:MET:N	2.11	0.65
1:A:399:LEU:HD12	1:A:554:TYR:HE1	1.60	0.65
1:A:776:PRO:HD2	1:A:779:ILE:O	1.95	0.65
1:B:363:GLU:HA	1:B:366:LEU:HD23	1.76	0.65
1:B:351:LEU:HD22	1:B:351:LEU:H	1.62	0.65
1:A:677:LEU:HD11	1:A:700:GLY:CA	2.28	0.64
1:B:743:PHE:O	1:B:744:LEU:HD23	1.98	0.64
1:A:409:ASP:HB3	1:A:412:HIS:CE1	2.32	0.64
1:A:629:THR:HB	1:A:672:LEU:HG	1.78	0.64
1:A:335:PHE:CD1	1:A:357:TRP:HZ3	2.14	0.64
1:A:827:ILE:HG23	1:A:828:LEU:HG	1.79	0.64
1:A:552:TYR:C	1:A:552:TYR:CD2	2.75	0.64
1:A:578:MET:C	1:A:582:MET:HE3	2.24	0.63
1:B:311:SER:CB	1:B:314:GLU:HG3	2.15	0.63
1:B:360:MET:HE3	1:B:361:ASP:N	2.12	0.63
1:A:595:ARG:HG3	1:A:595:ARG:HH11	1.62	0.63
1:A:657:ASP:OD2	1:A:657:ASP:C	2.41	0.63
1:B:558:GLU:HB2	1:B:576:TYR:CD1	2.33	0.63
1:B:575:MET:C	1:B:575:MET:HE2	2.23	0.63
1:B:645:ASN:OD1	1:B:645:ASN:C	2.41	0.63
1:B:716:MET:HG2	1:B:878:MET:HE2	1.81	0.63
1:A:819:LEU:CD1	1:A:845:MET:HE3	2.29	0.62
1:A:549:ASN:C	1:A:549:ASN:ND2	2.57	0.62
1:B:311:SER:HB2	1:B:314:GLU:HB2	1.81	0.62
1:A:319:TRP:CD1	1:A:322:ARG:HH21	2.17	0.62
1:A:363:GLU:H	1:A:363:GLU:CD	2.07	0.62
1:A:591:ASN:ND2	1:A:594:LEU:HD12	2.14	0.62
1:A:728:LYS:O	1:A:818:LYS:HD3	1.98	0.62
1:A:803:VAL:CG1	1:A:806:ARG:HD3	2.30	0.61
1:A:814:THR:HG22	1:A:818:LYS:O	2.00	0.61
1:A:842:SER:OG	1:A:844:GLU:OE1	2.18	0.61
1:B:397:TYR:N	1:B:397:TYR:CD1	2.65	0.61
1:B:810:ASN:O	1:B:822:ILE:HG22	2.00	0.61
1:A:716:MET:HG2	1:A:878:MET:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:GLU:HG2	1:B:410:PRO:HD3	1.83	0.61
1:B:838:PRO:HB2	1:B:924:LEU:HD12	1.83	0.61
1:B:667:PRO:O	1:B:670:THR:HG22	2.00	0.61
1:A:751:THR:CG2	1:A:754:GLU:CD	2.74	0.60
1:B:934:PRO:O	1:B:938:GLU:CG	2.48	0.60
1:A:668:MET:SD	1:A:668:MET:N	2.71	0.60
1:A:857:HIS:NE2	1:A:861:ARG:HD2	2.15	0.60
1:B:751:THR:HA	1:B:812:LEU:HD12	1.83	0.60
1:A:400:GLN:HG2	1:A:881:LEU:HD22	1.84	0.60
1:A:649:PHE:HE1	1:A:662:ILE:HG13	1.66	0.60
1:A:551:PHE:CE1	1:A:555:LEU:HD11	2.37	0.59
1:A:678:MET:O	1:A:699:HIS:CE1	2.55	0.59
1:B:807:HIS:HD2	1:B:809:ASP:H	1.50	0.59
1:B:326:SER:HA	1:B:357:TRP:CZ2	2.37	0.59
1:B:403:GLN:O	1:B:406:LYS:CB	2.49	0.59
1:B:913:THR:OG1	1:B:916:GLU:HG3	2.02	0.59
1:A:673:PHE:HB2	1:A:679:PRO:HD2	1.84	0.59
1:A:751:THR:HG23	1:A:754:GLU:HG3	1.83	0.59
1:A:854:SER:HB2	1:A:857:HIS:N	2.14	0.59
1:B:723:GLU:C	1:B:724:ASN:OD1	2.45	0.59
1:A:573:HIS:C	1:A:573:HIS:CD2	2.80	0.59
1:B:797:ILE:HG23	1:B:801:LEU:HD12	1.84	0.59
1:B:614:LEU:HD12	1:B:614:LEU:C	2.28	0.59
1:A:727:LEU:HB2	1:A:729:LEU:CD2	2.33	0.59
1:B:606:ARG:HH12	1:B:643:LYS:CG	2.16	0.59
1:B:343:LEU:HG	1:B:344:GLU:H	1.68	0.59
1:B:629:THR:HG22	1:B:672:LEU:CB	2.27	0.59
1:B:812:LEU:HD22	1:B:822:ILE:HB	1.85	0.59
1:A:862:LYS:O	1:A:866:THR:HG23	2.02	0.58
1:B:360:MET:HE3	1:B:360:MET:HA	1.85	0.58
1:B:846:VAL:HA	1:B:849:MET:HG3	1.85	0.58
1:A:399:LEU:CD1	1:A:554:TYR:HE1	2.15	0.58
1:A:532:ASN:OD1	1:A:535:THR:HG23	2.03	0.58
1:B:336:LEU:HB3	1:B:373:PHE:HE1	1.69	0.58
1:B:397:TYR:N	1:B:397:TYR:HD1	2.01	0.58
1:B:590:GLY:O	1:B:595:ARG:HD2	2.04	0.58
1:A:783:VAL:HG13	1:A:816:ASN:O	2.03	0.58
1:B:557:ILE:O	1:B:560:GLU:HG2	2.04	0.58
1:A:657:ASP:OD2	1:A:659:GLU:N	2.31	0.58
1:A:412:HIS:CB	1:A:532:ASN:ND2	2.66	0.58
1:B:738:SER:HB3	1:B:741:HIS:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:VAL:O	1:B:351:LEU:HD21	2.02	0.57
1:B:876:ASN:ND2	1:B:876:ASN:H	2.00	0.57
1:A:737:THR:O	1:A:738:SER:C	2.48	0.57
1:B:600:ASN:HA	1:B:603:LYS:HD3	1.86	0.57
1:B:405:LEU:C	1:B:405:LEU:HD23	2.30	0.57
1:B:728:LYS:HZ3	1:B:786:THR:HG22	1.69	0.57
1:B:665:ILE:HG22	1:B:666:VAL:N	2.20	0.57
1:A:806:ARG:HD2	1:A:806:ARG:N	2.20	0.57
1:A:944:THR:OG1	1:B:931:ALA:O	2.15	0.57
1:B:367:GLU:HG2	1:B:880:ASN:OD1	2.03	0.57
1:B:335:PHE:CD1	1:B:357:TRP:CZ3	2.93	0.57
1:A:306:PRO:HG3	1:A:876:ASN:HA	1.87	0.57
1:B:403:GLN:O	1:B:406:LYS:HB3	2.05	0.57
1:B:595:ARG:HH11	1:B:595:ARG:CG	1.98	0.57
1:A:712:MET:O	1:A:716:MET:HG3	2.05	0.56
1:A:811:LEU:N	1:A:811:LEU:CD2	2.67	0.56
1:A:830:ARG:HH22	1:A:903:LYS:NZ	2.01	0.56
1:A:835:MET:HE3	1:B:942:ARG:HD3	1.85	0.56
1:B:682:LEU:HD23	1:B:684:PHE:CE2	2.36	0.56
1:A:776:PRO:HG2	1:A:777:TYR:N	2.20	0.56
1:A:363:GLU:HA	1:A:366:LEU:HD12	1.86	0.56
1:A:776:PRO:HG2	1:A:777:TYR:H	1.71	0.56
1:A:819:LEU:HD23	1:A:819:LEU:O	2.06	0.56
1:A:883:SER:O	1:A:886:VAL:HG23	2.06	0.56
1:B:380:LYS:HD2	1:B:380:LYS:C	2.31	0.56
1:A:649:PHE:CZ	1:A:663:THR:O	2.59	0.56
1:A:812:LEU:HD12	1:A:820:PHE:CZ	2.40	0.56
1:A:677:LEU:CD1	1:A:700:GLY:HA3	2.35	0.56
1:A:302:TYR:HE1	1:A:331:ALA:CB	2.19	0.55
1:B:768:LYS:HE2	1:B:769:HIS:NE2	2.20	0.55
1:A:549:ASN:HD22	1:A:550:TYR:N	2.04	0.55
1:A:701:ASP:O	1:A:740:LYS:HA	2.07	0.55
1:B:909:GLN:HG3	1:B:912:LEU:HG	1.87	0.55
1:A:533:LEU:O	1:A:536:PHE:HB3	2.07	0.55
1:A:645:ASN:O	1:A:648:ASN:O	2.24	0.55
1:B:603:LYS:HB3	1:B:652:ILE:HD11	1.88	0.55
1:B:304:TYR:CB	1:B:305:PRO:CD	2.84	0.55
1:A:553:TRP:O	1:A:557:ILE:HG13	2.07	0.55
1:B:776:PRO:HB2	1:B:777:TYR:HD1	1.72	0.55
1:B:920:HIS:C	1:B:920:HIS:CD2	2.85	0.55
1:B:304:TYR:HB2	1:B:305:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:HIS:ND1	1:B:741:HIS:N	2.55	0.55
1:A:326:SER:HB2	1:A:357:TRP:CE2	2.42	0.54
1:A:830:ARG:HH22	1:A:903:LYS:HZ1	1.53	0.54
1:A:307:THR:OG1	1:A:905:GLU:OE2	2.26	0.54
1:A:549:ASN:C	1:A:549:ASN:HD22	2.15	0.54
1:A:909:GLN:HG3	1:A:912:LEU:HG	1.88	0.54
1:B:806:ARG:N	1:B:806:ARG:HD2	2.22	0.54
1:B:827:ILE:HG23	1:B:828:LEU:HG	1.89	0.54
1:A:591:ASN:HD21	1:A:594:LEU:HD12	1.72	0.54
1:A:550:TYR:HB3	1:A:554:TYR:HE2	1.72	0.54
1:A:913:THR:HG23	1:A:916:GLU:H	1.72	0.54
1:B:311:SER:CB	1:B:314:GLU:HB2	2.36	0.54
1:B:661:TYR:O	1:B:686:THR:HA	2.08	0.54
1:B:667:PRO:O	1:B:670:THR:CG2	2.55	0.54
1:A:291:ALA:O	1:A:294:ARG:HG2	2.08	0.54
1:A:723:GLU:O	1:A:724:ASN:CB	2.55	0.54
1:B:865:TYR:HD1	1:B:918:VAL:HG13	1.67	0.54
1:A:723:GLU:OE1	1:A:723:GLU:HA	2.08	0.53
1:B:838:PRO:HB2	1:B:924:LEU:CD1	2.38	0.53
1:A:678:MET:O	1:A:699:HIS:NE2	2.42	0.53
1:A:343:LEU:HB3	1:A:346:GLU:HG2	1.89	0.53
1:B:719:LEU:O	1:B:723:GLU:HG2	2.09	0.53
1:A:292:SER:CB	1:A:292:SER:HG	2.09	0.53
1:A:575:MET:O	1:A:579:VAL:HG23	2.08	0.53
1:B:813:LEU:CD1	1:B:818:LYS:O	2.53	0.53
1:B:926:ASP:O	1:B:930:THR:HG23	2.08	0.53
1:B:314:GLU:CA	1:B:317:LEU:HG	2.26	0.53
1:A:726:ASP:C	1:A:727:LEU:HD23	2.33	0.53
1:B:803:VAL:HG12	1:B:806:ARG:HD3	1.90	0.53
1:A:370:SER:O	1:A:379:ARG:NH2	2.41	0.53
1:A:702:ASP:OD2	1:A:702:ASP:C	2.52	0.53
1:B:594:LEU:N	1:B:594:LEU:HD23	2.24	0.53
1:A:335:PHE:C	1:A:335:PHE:CD2	2.87	0.53
1:B:712:MET:HE1	1:B:878:MET:HG2	1.91	0.53
1:B:859:GLU:OE1	1:B:859:GLU:HA	2.08	0.53
1:A:737:THR:CG2	1:A:738:SER:N	2.71	0.53
1:A:561:GLU:N	1:A:561:GLU:CD	2.67	0.52
1:A:729:LEU:HD23	1:A:729:LEU:N	2.24	0.52
1:A:728:LYS:HG3	1:A:786:THR:HB	1.92	0.52
1:A:632:PHE:HE1	1:A:636:LEU:HD21	1.75	0.52
1:B:381:TYR:O	1:B:384:SER:OG	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LEU:HD22	1:A:345:ASP:H	1.73	0.52
1:B:948:ARG:HH11	1:B:948:ARG:CG	2.22	0.52
1:A:294:ARG:HD2	1:A:321:PHE:CE1	2.45	0.52
1:B:763:HIS:HE2	1:B:848:ALA:C	2.18	0.52
1:B:790:SER:HB2	1:B:819:LEU:H	1.74	0.52
1:A:756:LEU:CD1	1:A:844:GLU:HG2	2.35	0.52
1:B:568:GLN:HE22	1:B:571:ARG:HH11	1.58	0.52
1:A:766:PHE:CE1	1:A:813:LEU:HD12	2.44	0.52
1:B:385:ARG:HA	1:B:385:ARG:NE	2.23	0.52
1:B:746:TYR:C	1:B:746:TYR:CD2	2.87	0.52
1:A:399:LEU:CD1	1:A:554:TYR:CE1	2.89	0.52
1:A:806:ARG:NH2	1:A:822:ILE:O	2.33	0.52
1:B:782:GLU:O	1:B:786:THR:HG23	2.09	0.52
1:A:708:LEU:HD12	1:A:885:MET:HE2	1.92	0.51
1:A:811:LEU:C	1:A:812:LEU:HD23	2.35	0.51
1:A:561:GLU:CD	1:A:561:GLU:H	2.16	0.51
1:A:602:ARG:NH2	1:A:606:ARG:HD2	2.25	0.51
1:B:364:ASP:O	1:B:367:GLU:HB2	2.09	0.51
1:B:595:ARG:NH1	1:B:595:ARG:CG	2.66	0.51
1:B:679:PRO:HB3	1:B:698:LYS:HG3	1.92	0.51
1:B:300:ILE:HA	1:B:304:TYR:HD2	1.76	0.51
1:B:656:LEU:HD12	1:B:743:PHE:HB3	1.93	0.51
1:B:763:HIS:CE1	1:B:777:TYR:CD2	2.99	0.51
1:B:297:LEU:O	1:B:300:ILE:HG12	2.10	0.51
1:B:732:TYR:HB2	1:B:745:GLN:HB3	1.93	0.51
1:A:304:TYR:CB	1:A:305:PRO:HD3	2.41	0.51
1:A:696:ILE:HG22	1:A:697:PHE:N	2.25	0.51
1:B:698:LYS:O	1:B:741:HIS:HA	2.11	0.51
1:B:914:ASP:OD1	1:B:914:ASP:N	2.44	0.51
1:A:409:ASP:OD1	1:A:411:ARG:N	2.42	0.51
1:B:360:MET:HE2	1:B:364:ASP:CB	2.40	0.51
1:B:400:GLN:HG2	1:B:881:LEU:HD13	1.92	0.51
1:B:592:PHE:N	1:B:595:ARG:HE	2.08	0.51
1:B:812:LEU:CD2	1:B:822:ILE:HB	2.40	0.51
1:A:559:VAL:HG22	1:A:577:ALA:HA	1.93	0.51
1:A:677:LEU:CD1	1:A:700:GLY:CA	2.89	0.51
1:B:351:LEU:HA	1:B:354:LEU:HB3	1.92	0.51
1:B:573:HIS:C	1:B:573:HIS:CD2	2.89	0.51
1:B:664:LYS:HG3	1:B:685:VAL:CG2	2.41	0.51
1:A:326:SER:O	1:A:326:SER:OG	2.27	0.51
1:B:575:MET:HE2	1:B:575:MET:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:MET:HE2	1:B:576:TYR:HA	1.93	0.50
1:B:582:MET:O	1:B:586:VAL:HG23	2.10	0.50
1:A:776:PRO:HG3	1:A:784:MET:HG3	1.92	0.50
1:A:293:ILE:O	1:A:297:LEU:HG	2.12	0.50
1:A:610:GLU:OE1	1:A:643:LYS:CB	2.56	0.50
1:A:866:THR:O	1:A:870:HIS:HD2	1.94	0.50
1:B:624:ASN:OD1	1:B:625:ARG:N	2.44	0.50
1:B:823:ASP:OD1	1:B:824:PHE:N	2.45	0.50
1:B:776:PRO:HB2	1:B:777:TYR:CD1	2.46	0.50
1:A:610:GLU:OE1	1:A:643:LYS:N	2.45	0.50
1:B:698:LYS:HZ1	2:B:1950:090:HAW	1.75	0.50
1:A:723:GLU:OE1	1:A:723:GLU:CA	2.60	0.50
1:A:772:CYS:O	1:A:778:GLY:HA2	2.12	0.50
1:A:805:ASP:N	1:A:831:ASP:OD2	2.45	0.50
1:B:888:ALA:O	1:B:889:THR:HB	2.12	0.50
1:A:595:ARG:HG3	1:A:595:ARG:NH1	2.27	0.49
1:B:751:THR:OG1	1:B:809:ASP:HA	2.12	0.49
1:B:885:MET:O	1:B:888:ALA:HB2	2.11	0.49
1:A:640:ASP:OD2	1:A:640:ASP:N	2.45	0.49
1:B:363:GLU:HG2	1:B:877:VAL:HG22	1.95	0.49
1:B:888:ALA:O	1:B:889:THR:CB	2.59	0.49
1:A:375:HIS:HD2	1:A:377:GLN:HB3	1.77	0.49
1:A:341:TRP:CD1	1:A:342:LYS:HG2	2.47	0.49
1:B:394:LEU:O	1:B:398:LEU:HB2	2.11	0.49
1:A:743:PHE:O	1:A:744:LEU:HD23	2.11	0.49
1:B:558:GLU:HB2	1:B:576:TYR:HD1	1.76	0.49
1:A:761:ASN:OD1	1:A:764:ASN:ND2	2.45	0.49
1:A:332:LEU:HD12	1:A:336:LEU:CD2	2.43	0.49
1:A:763:HIS:HE1	1:A:777:TYR:CE2	2.31	0.49
1:B:606:ARG:HH12	1:B:643:LYS:HG3	1.76	0.49
1:B:763:HIS:HE1	1:B:777:TYR:CD2	2.30	0.49
1:B:862:LYS:O	1:B:866:THR:HG23	2.12	0.49
1:A:649:PHE:CE2	1:A:663:THR:O	2.65	0.49
1:A:710:LEU:HD22	1:A:732:TYR:O	2.13	0.49
1:B:657:ASP:OD2	1:B:657:ASP:C	2.55	0.49
1:B:698:LYS:HZ2	2:B:1950:090:HAW	1.78	0.49
1:B:720:LEU:O	1:B:723:GLU:HB2	2.13	0.49
1:B:304:TYR:HB2	1:B:305:PRO:HD2	1.95	0.49
1:A:400:GLN:HG2	1:A:881:LEU:CD2	2.43	0.49
1:A:807:HIS:H	1:A:810:ASN:HB2	1.78	0.49
1:A:943:PHE:HB2	1:B:931:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:SER:CB	1:B:819:LEU:H	2.26	0.48
1:B:826:TYR:HB3	1:B:830:ARG:O	2.13	0.48
1:A:300:ILE:O	1:A:304:TYR:HB2	2.13	0.48
1:A:302:TYR:HE1	1:A:331:ALA:HB2	1.78	0.48
1:B:315:GLN:HG3	1:B:316:ASP:N	2.28	0.48
1:B:724:ASN:OD1	1:B:724:ASN:N	2.46	0.48
1:A:362:VAL:O	1:A:366:LEU:HD12	2.13	0.48
1:A:582:MET:O	1:A:586:VAL:HG23	2.13	0.48
1:A:677:LEU:CD1	1:A:700:GLY:N	2.61	0.48
1:A:854:SER:C	1:A:856:HIS:N	2.68	0.48
1:B:822:ILE:HD11	2:B:1950:090:OAU	2.13	0.48
1:B:822:ILE:CD1	2:B:1950:090:CAM	2.91	0.48
1:B:408:GLU:HB3	1:B:410:PRO:HD3	1.96	0.48
1:A:411:ARG:HA	1:A:414:VAL:CG2	2.43	0.48
1:A:846:VAL:HB	1:A:933:MET:HE1	1.96	0.48
1:A:920:HIS:O	1:A:923:SER:HB3	2.13	0.48
1:A:302:TYR:CE1	1:A:331:ALA:CB	2.97	0.48
1:A:332:LEU:HD12	1:A:336:LEU:HD23	1.95	0.48
1:A:819:LEU:HD11	1:A:845:MET:HE3	1.94	0.48
1:A:708:LEU:HD23	1:A:708:LEU:O	2.14	0.48
1:A:405:LEU:HD23	1:A:533:LEU:HD21	1.96	0.48
1:A:777:TYR:N	1:A:777:TYR:CD1	2.81	0.48
1:A:371:PRO:HG3	1:A:407:TYR:CZ	2.48	0.47
1:A:708:LEU:C	1:A:708:LEU:CD2	2.85	0.47
1:A:779:ILE:O	1:A:780:SER:C	2.56	0.47
1:B:300:ILE:HA	1:B:304:TYR:CD2	2.49	0.47
1:B:295:ASP:O	1:B:299:THR:HG23	2.14	0.47
1:B:654:PHE:CD1	1:B:655:PRO:HD2	2.48	0.47
1:A:913:THR:HG22	1:A:916:GLU:CG	2.44	0.47
1:A:925:LEU:O	1:A:929:ILE:HG13	2.14	0.47
1:B:702:ASP:OD1	1:B:704:ARG:NH2	2.47	0.47
1:A:673:PHE:HD2	1:A:679:PRO:HG2	1.79	0.47
1:A:305:PRO:HG2	1:A:308:TYR:CD1	2.49	0.47
1:A:852:ILE:N	1:A:852:ILE:CD1	2.77	0.47
1:A:587:LEU:HB3	1:A:598:PHE:HB2	1.97	0.47
1:B:335:PHE:CD1	1:B:357:TRP:HZ3	2.32	0.47
1:B:703:LEU:CD2	1:B:744:LEU:HD21	2.44	0.47
1:B:350:ALA:O	1:B:353:MET:HB2	2.14	0.47
1:A:313:GLU:CA	1:A:313:GLU:OE1	2.63	0.47
1:B:624:ASN:H	1:B:627:LYS:HD2	1.80	0.47
1:A:677:LEU:HD11	1:A:700:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:TRP:CD1	1:B:322:ARG:HD2	2.50	0.47
1:A:373:PHE:N	1:A:373:PHE:CD2	2.83	0.46
1:B:829:GLY:O	1:B:830:ARG:C	2.54	0.46
1:A:663:THR:HG23	1:A:685:VAL:HG22	1.96	0.46
1:B:544:ASN:OD1	1:B:544:ASN:C	2.57	0.46
1:B:618:VAL:HG11	1:B:632:PHE:HD2	1.79	0.46
1:A:412:HIS:HB3	1:A:532:ASN:HD21	1.74	0.46
1:A:651:PRO:HA	1:A:662:ILE:O	2.15	0.46
1:A:739:SER:O	1:A:740:LYS:CG	2.61	0.46
1:B:661:TYR:HB3	1:B:687:SER:HB3	1.97	0.46
1:B:763:HIS:NE2	1:B:848:ALA:O	2.39	0.46
1:B:861:ARG:O	1:B:865:TYR:CD2	2.68	0.46
1:A:416:LEU:CD1	1:A:535:THR:HG22	2.42	0.46
1:A:727:LEU:O	1:A:729:LEU:N	2.46	0.46
1:A:913:THR:HG22	1:A:916:GLU:HB2	1.97	0.46
1:A:648:ASN:HA	1:A:664:LYS:HG2	1.97	0.46
1:B:342:LYS:HG3	1:B:343:LEU:HD23	1.97	0.46
1:B:408:GLU:CB	1:B:409:ASP:HA	2.26	0.46
1:B:549:ASN:HD22	1:B:550:TYR:N	2.13	0.46
1:A:737:THR:HG21	1:A:741:HIS:CD2	2.50	0.46
1:A:814:THR:CG2	1:A:818:LYS:N	2.69	0.46
1:B:777:TYR:O	1:B:779:ILE:N	2.48	0.46
1:B:861:ARG:HB3	1:B:865:TYR:HE2	1.81	0.46
1:A:649:PHE:CE1	1:A:663:THR:O	2.68	0.46
1:A:607:PHE:CD1	1:A:607:PHE:C	2.95	0.46
1:B:648:ASN:HA	1:B:664:LYS:HB3	1.98	0.46
1:A:553:TRP:CZ3	1:A:737:THR:HG23	2.51	0.45
1:A:677:LEU:CG	1:A:700:GLY:HA3	2.45	0.45
1:A:720:LEU:HD23	1:A:720:LEU:N	2.30	0.45
1:A:805:ASP:O	1:A:810:ASN:ND2	2.48	0.45
1:B:360:MET:HA	1:B:360:MET:CE	2.44	0.45
1:A:330:LYS:O	1:A:333:THR:HG23	2.15	0.45
1:A:717:ASP:OD2	1:A:721:ARG:NH1	2.48	0.45
1:A:766:PHE:HE1	1:A:813:LEU:HD12	1.81	0.45
1:B:816:ASN:OD1	1:B:816:ASN:O	2.33	0.45
1:B:822:ILE:HD11	2:B:1950:090:NAN	2.31	0.45
1:B:842:SER:O	1:B:846:VAL:HG23	2.15	0.45
1:A:591:ASN:O	1:A:595:ARG:NH1	2.50	0.45
1:A:812:LEU:O	1:A:819:LEU:HA	2.16	0.45
1:A:544:ASN:C	1:A:544:ASN:OD1	2.59	0.45
1:B:610:GLU:OE1	1:B:643:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:GLY:O	1:B:854:SER:HB2	2.16	0.45
1:B:863:GLN:OE1	1:B:863:GLN:HA	2.15	0.45
1:A:677:LEU:HG	1:A:700:GLY:HA3	1.98	0.45
1:B:360:MET:HE3	1:B:360:MET:CA	2.45	0.45
1:B:723:GLU:O	1:B:724:ASN:OD1	2.34	0.45
1:A:677:LEU:HB3	1:A:698:LYS:HE3	1.98	0.45
1:A:785:ASP:O	1:A:789:LYS:HG3	2.17	0.45
1:B:587:LEU:HB3	1:B:598:PHE:HB2	1.99	0.45
1:B:629:THR:O	1:B:633:GLN:HG3	2.15	0.45
1:B:612:VAL:CG2	1:B:741:HIS:HD2	2.29	0.45
1:B:744:LEU:O	1:B:745:GLN:C	2.58	0.45
1:A:671:SER:C	1:A:672:LEU:HD23	2.42	0.45
1:B:363:GLU:N	1:B:363:GLU:OE2	2.50	0.45
1:B:408:GLU:CB	1:B:410:PRO:HD3	2.47	0.45
1:B:558:GLU:HG3	1:B:576:TYR:CE1	2.52	0.45
1:A:368:LEU:HD22	1:A:373:PHE:CE1	2.52	0.44
1:B:682:LEU:HD22	1:B:682:LEU:N	2.22	0.44
1:B:306:PRO:O	1:B:307:THR:HG23	2.17	0.44
1:B:558:GLU:HG3	1:B:576:TYR:HE1	1.82	0.44
1:B:672:LEU:HD22	1:B:678:MET:HB2	2.00	0.44
1:A:305:PRO:HG2	1:A:308:TYR:CG	2.53	0.44
1:A:763:HIS:CE1	1:A:777:TYR:CD2	3.05	0.44
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.71	0.44
1:A:715:LEU:HD23	1:A:716:MET:N	2.33	0.44
1:B:751:THR:HG23	1:B:754:GLU:H	1.83	0.44
1:A:747:VAL:CG2	1:A:820:PHE:CZ	3.00	0.44
1:B:296:GLN:O	1:B:300:ILE:HG23	2.18	0.44
1:B:308:TYR:CD1	1:B:310:LEU:HB2	2.53	0.44
1:B:380:LYS:HZ1	1:B:381:TYR:HB2	1.83	0.44
1:B:557:ILE:HD11	1:B:736:ALA:O	2.18	0.44
1:B:704:ARG:CZ	1:B:889:THR:HG21	2.46	0.44
1:A:302:TYR:CE1	1:A:331:ALA:HB2	2.52	0.44
1:A:552:TYR:CG	1:A:601:LEU:HD22	2.52	0.44
1:B:672:LEU:HD23	1:B:679:PRO:O	2.18	0.44
1:A:341:TRP:NE1	1:A:342:LYS:HG2	2.32	0.43
1:A:593:ASN:O	1:A:597:ILE:HG13	2.18	0.43
1:A:671:SER:O	1:A:672:LEU:HD23	2.17	0.43
1:A:674:LYS:H	1:A:674:LYS:CD	2.26	0.43
1:A:727:LEU:N	1:A:727:LEU:CD2	2.69	0.43
1:B:403:GLN:O	1:B:406:LYS:HB2	2.18	0.43
1:A:342:LYS:HD3	1:A:342:LYS:HA	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:LEU:HD21	1:A:822:ILE:HD12	2.01	0.43
1:B:364:ASP:OD2	1:B:365:ALA:N	2.51	0.43
1:B:656:LEU:C	1:B:656:LEU:CD2	2.90	0.43
1:A:318:VAL:O	1:A:322:ARG:HB3	2.17	0.43
1:A:398:LEU:C	1:A:398:LEU:HD13	2.43	0.43
1:B:311:SER:OG	1:B:314:GLU:HB2	2.19	0.43
1:B:375:HIS:CD2	1:B:377:GLN:H	2.36	0.43
1:A:776:PRO:CG	1:A:777:TYR:N	2.81	0.43
1:B:734:VAL:HG13	1:B:744:LEU:CD2	2.49	0.43
1:A:662:ILE:H	1:A:662:ILE:HG12	1.67	0.43
1:B:763:HIS:CD2	1:B:848:ALA:HA	2.54	0.43
1:A:677:LEU:HD21	1:A:699:HIS:HD2	1.84	0.43
1:B:319:TRP:HA	1:B:322:ARG:HB3	2.01	0.43
1:B:336:LEU:HB3	1:B:373:PHE:CE1	2.50	0.43
1:A:625:ARG:NH2	1:A:674:LYS:HA	2.29	0.43
1:A:638:GLU:HG2	1:A:641:MET:SD	2.59	0.43
1:A:885:MET:O	1:A:888:ALA:HB2	2.19	0.43
2:A:1949:090:OAU	2:A:1949:090:NAL	2.52	0.43
1:B:824:PHE:HB3	1:B:827:ILE:HD11	2.01	0.43
1:A:672:LEU:HD12	1:A:678:MET:CE	2.49	0.43
1:A:766:PHE:CZ	1:A:813:LEU:HD11	2.53	0.43
1:A:822:ILE:HD13	1:A:822:ILE:HG21	1.80	0.43
1:B:631:LYS:O	1:B:635:LEU:HD23	2.18	0.43
1:B:823:ASP:OD1	1:B:823:ASP:C	2.62	0.43
1:A:737:THR:CG2	1:A:741:HIS:CD2	3.02	0.43
1:B:322:ARG:HD3	1:B:335:PHE:CD1	2.53	0.43
1:B:408:GLU:CG	1:B:410:PRO:HD3	2.49	0.43
1:B:591:ASN:O	1:B:593:ASN:N	2.52	0.43
1:B:618:VAL:HG22	1:B:631:LYS:HG3	1.99	0.43
1:B:912:LEU:HD12	1:B:917:ALA:HA	2.00	0.43
1:A:766:PHE:HZ	1:A:813:LEU:HD11	1.83	0.42
1:B:304:TYR:O	1:B:305:PRO:C	2.62	0.42
1:B:382:ALA:O	1:B:385:ARG:HB2	2.19	0.42
1:B:660:ILE:HG23	1:B:686:THR:HG23	2.01	0.42
1:B:804:GLY:O	1:B:805:ASP:HB3	2.19	0.42
1:B:822:ILE:HG23	1:B:823:ASP:N	2.33	0.42
1:A:621:GLU:HA	1:A:622:PRO:HD3	1.90	0.42
1:A:684:PHE:CD2	1:A:684:PHE:N	2.87	0.42
1:B:551:PHE:CE1	1:B:555:LEU:HD21	2.55	0.42
1:B:751:THR:CA	1:B:812:LEU:HD12	2.49	0.42
1:B:841:LEU:O	1:B:932:VAL:HG21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:SER:OG	1:A:292:SER:CA	2.56	0.42
1:A:602:ARG:NH1	1:A:606:ARG:HD2	2.34	0.42
1:A:610:GLU:HG3	1:A:644:VAL:HG12	2.02	0.42
1:A:830:ARG:NH2	1:A:903:LYS:HZ1	2.17	0.42
1:B:682:LEU:H	1:B:682:LEU:CD2	2.26	0.42
1:A:806:ARG:NH2	1:A:810:ASN:HB3	2.33	0.42
1:A:914:ASP:OD1	1:A:914:ASP:N	2.52	0.42
1:B:370:SER:HB2	1:B:371:PRO:CD	2.49	0.42
1:B:678:MET:HA	1:B:679:PRO:HD3	1.85	0.42
1:A:650:GLU:HA	1:A:651:PRO:HD3	1.88	0.42
1:A:846:VAL:HB	1:A:933:MET:CE	2.49	0.42
1:B:734:VAL:CG2	1:B:744:LEU:HD22	2.43	0.42
1:B:828:LEU:N	1:B:828:LEU:HD23	2.34	0.42
1:A:677:LEU:CD1	1:A:698:LYS:HE3	2.50	0.42
1:B:605:ARG:O	1:B:606:ARG:C	2.61	0.42
1:B:710:LEU:HD22	1:B:732:TYR:O	2.19	0.42
1:B:729:LEU:N	1:B:729:LEU:HD23	2.35	0.42
1:B:870:HIS:O	1:B:873:ARG:HB2	2.20	0.42
1:A:343:LEU:CB	1:A:346:GLU:HG2	2.48	0.42
1:A:363:GLU:CD	1:A:363:GLU:N	2.77	0.42
1:A:657:ASP:HA	1:A:658:PRO:HD3	1.86	0.42
1:A:763:HIS:NE2	1:A:848:ALA:O	2.35	0.42
1:B:603:LYS:HE3	1:B:652:ILE:HG12	2.02	0.42
1:A:747:VAL:HG22	2:A:1949:090:HAA	1.85	0.42
1:A:805:ASP:O	1:A:805:ASP:CG	2.63	0.42
1:B:614:LEU:HD23	1:B:646:PHE:CE1	2.55	0.42
1:A:719:LEU:HD23	1:A:719:LEU:HA	1.81	0.42
1:A:719:LEU:O	1:A:723:GLU:HG2	2.20	0.42
1:A:830:ARG:NH2	1:A:903:LYS:NZ	2.68	0.42
1:B:360:MET:HG3	1:B:364:ASP:CG	2.44	0.42
1:B:591:ASN:O	1:B:592:PHE:C	2.63	0.42
1:B:888:ALA:O	1:B:889:THR:HG22	2.20	0.42
1:A:296:GLN:OE1	1:A:296:GLN:HA	2.20	0.41
1:B:766:PHE:CZ	1:B:817:GLY:HA2	2.55	0.41
1:A:318:VAL:O	1:A:322:ARG:CB	2.68	0.41
1:A:552:TYR:CD1	1:A:601:LEU:HD22	2.54	0.41
1:B:948:ARG:CG	1:B:948:ARG:NH1	2.83	0.41
1:A:661:TYR:O	1:A:686:THR:HB	2.20	0.41
1:A:663:THR:HG23	1:A:685:VAL:CG2	2.51	0.41
1:A:922:GLN:HE22	1:B:919:GLN:CB	2.30	0.41
1:B:661:TYR:CB	1:B:687:SER:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:PHE:C	1:B:744:LEU:HD23	2.45	0.41
1:A:363:GLU:HA	1:A:366:LEU:HD13	2.00	0.41
1:B:701:ASP:C	1:B:740:LYS:HA	2.46	0.41
1:B:363:GLU:O	1:B:364:ASP:C	2.62	0.41
1:A:319:TRP:CD1	1:A:322:ARG:NH2	2.85	0.41
1:A:335:PHE:CD2	1:A:335:PHE:O	2.73	0.41
1:A:533:LEU:HD23	1:A:534:CYS:N	2.34	0.41
1:B:339:ILE:H	1:B:339:ILE:HG13	1.66	0.41
1:A:634:LYS:O	1:A:634:LYS:CE	2.67	0.41
1:B:409:ASP:OD1	1:B:410:PRO:HD2	2.20	0.41
1:B:718:LYS:O	1:B:722:ARG:HG3	2.20	0.41
1:B:748:ASP:OD2	1:B:748:ASP:C	2.64	0.41
1:B:822:ILE:CD1	2:B:1950:090:NAL	2.77	0.41
1:A:624:ASN:O	1:A:625:ARG:C	2.64	0.41
1:A:712:MET:HE3	1:A:716:MET:HE3	2.01	0.41
1:A:776:PRO:HG2	1:A:777:TYR:CD1	2.33	0.41
1:B:320:LYS:HG3	1:B:321:PHE:N	2.34	0.41
1:A:584:LEU:HD23	1:A:584:LEU:HA	1.91	0.41
1:A:804:GLY:HA3	1:A:831:ASP:OD2	2.21	0.41
1:A:822:ILE:HD13	2:A:1949:090:CAM	2.51	0.41
1:B:375:HIS:HB3	1:B:378:VAL:HG22	2.03	0.41
1:B:420:ILE:O	1:B:420:ILE:HG22	2.19	0.41
1:B:533:LEU:C	1:B:533:LEU:HD13	2.45	0.41
1:B:614:LEU:HB2	1:B:642:PHE:CE1	2.56	0.41
1:A:417:HIS:HD2	1:A:578:MET:HG2	1.86	0.40
1:A:586:VAL:O	1:A:586:VAL:HG12	2.20	0.40
1:B:319:TRP:N	1:B:322:ARG:HH21	2.19	0.40
1:B:325:LEU:C	1:B:327:SER:H	2.28	0.40
1:B:843:LYS:HA	1:B:932:VAL:CG1	2.51	0.40
1:A:309:VAL:O	1:A:311:SER:N	2.54	0.40
1:A:405:LEU:HD23	1:A:533:LEU:CD2	2.51	0.40
1:B:598:PHE:CD2	1:B:598:PHE:C	2.98	0.40
1:B:908:LEU:HD23	1:B:908:LEU:HA	1.87	0.40
1:A:625:ARG:CG	1:A:626:ASN:N	2.81	0.40
1:A:758:ARG:HE	1:A:758:ARG:HB2	1.70	0.40
1:A:883:SER:O	1:A:886:VAL:CG2	2.70	0.40
1:A:373:PHE:N	1:A:373:PHE:HD2	2.19	0.40
1:A:538:ILE:O	1:A:542:CYS:SG	2.76	0.40
1:A:871:LEU:CD2	1:A:878:MET:HE1	2.42	0.40
1:B:330:LYS:NZ	1:B:334:LYS:HE2	2.37	0.40
1:B:549:ASN:ND2	1:B:549:ASN:C	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ASP:OD2	1:A:659:GLU:HB2	2.21	0.40
1:B:343:LEU:HD23	1:B:343:LEU:H	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	540/696 (78%)	504 (93%)	26 (5%)	10 (2%)	6	26
1	B	538/696 (77%)	503 (94%)	24 (4%)	11 (2%)	6	25
All	All	1078/1392 (77%)	1007 (93%)	50 (5%)	21 (2%)	6	26

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	LEU
1	B	592	PHE
1	B	778	GLY
1	A	305	PRO
1	A	310	LEU
1	A	327	SER
1	A	591	ASN
1	B	304	TYR
1	B	306	PRO
1	B	690	HIS
1	A	304	TYR
1	B	310	LEU
1	A	731	PRO
1	B	731	PRO
1	B	776	PRO
1	A	329	LYS

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Mol	Chain	Res	Type
1	A	675	SER
1	A	690	HIS
1	A	738	SER
1	B	805	ASP
1	B	305	PRO

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	491/612 (80%)	384 (78%)	107 (22%)	1	3
1	B	490/612 (80%)	387 (79%)	103 (21%)	1	4
All	All	981/1224 (80%)	771 (79%)	210 (21%)	1	3

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	294	ARG
1	A	296	GLN
1	A	309	VAL
1	A	310	LEU
1	A	313	GLU
1	A	318	VAL
1	A	322	ARG
1	A	325	LEU
1	A	329	LYS
1	A	333	THR
1	A	335	PHE
1	A	336	LEU
1	A	339	ILE
1	A	342	LYS
1	A	343	LEU
1	A	345	ASP
1	A	351	LEU
1	A	354	LEU

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Mol	Chain	Res	Type
1	A	363	GLU
1	A	366	LEU
1	A	370	SER
1	A	378	VAL
1	A	394	LEU
1	A	396	LEU
1	A	409	ASP
1	A	414	VAL
1	A	532	ASN
1	A	533	LEU
1	A	534	CYS
1	A	543	THR
1	A	546	THR
1	A	547	LEU
1	A	549	ASN
1	A	560	GLU
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	602	ARG
1	A	611	LEU
1	A	614	LEU
1	A	615	VAL
1	A	621	GLU
1	A	625	ARG
1	A	629	THR
1	A	634	LYS
1	A	639	GLN
1	A	640	ASP
1	A	643	LYS
1	A	645	ASN
1	A	649	PHE
1	A	656	LEU
1	A	659	GLU
1	A	662	ILE
1	A	666	VAL
1	A	668	MET
1	A	670	THR
1	A	671	SER

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Mol	Chain	Res	Type
1	A	674	LYS
1	A	677	LEU
1	A	682	LEU
1	A	685	VAL
1	A	686	THR
1	A	699	HIS
1	A	701	ASP
1	A	702	ASP
1	A	710	LEU
1	A	711	GLN
1	A	715	LEU
1	A	717	ASP
1	A	720	LEU
1	A	722	ARG
1	A	723	GLU
1	A	724	ASN
1	A	727	LEU
1	A	729	LEU
1	A	741	HIS
1	A	744	LEU
1	A	750	CYS
1	A	751	THR
1	A	759	GLU
1	A	786	THR
1	A	788	ILE
1	A	790	SER
1	A	808	LEU
1	A	811	LEU
1	A	812	LEU
1	A	813	LEU
1	A	814	THR
1	A	819	LEU
1	A	822	ILE
1	A	827	ILE
1	A	831	ASP
1	A	833	LYS
1	A	839	MET
1	A	852	ILE
1	A	859	GLU
1	A	862	LYS
1	A	883	SER
1	A	896	GLU

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Mol	Chain	Res	Type
1	A	902	LYS
1	A	912	LEU
1	A	927	VAL
1	A	940	ILE
1	A	945	GLN
1	B	294	ARG
1	B	301	VAL
1	B	308	TYR
1	B	309	VAL
1	B	313	GLU
1	B	314	GLU
1	B	317	LEU
1	B	318	VAL
1	B	321	PHE
1	B	325	LEU
1	B	327	SER
1	B	328	HIS
1	B	333	THR
1	B	339	ILE
1	B	346	GLU
1	B	351	LEU
1	B	354	LEU
1	B	363	GLU
1	B	364	ASP
1	B	367	GLU
1	B	374	THR
1	B	377	GLN
1	B	380	LYS
1	B	397	TYR
1	B	405	LEU
1	B	417	HIS
1	B	419	CYS
1	B	546	THR
1	B	547	LEU
1	B	549	ASN
1	B	568	GLN
1	B	571	ARG
1	B	573	HIS
1	B	575	MET
1	B	580	LEU
1	B	586	VAL
1	B	594	LEU

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Mol	Chain	Res	Type
1	B	595	ARG
1	B	606	ARG
1	B	611	LEU
1	B	612	VAL
1	B	614	LEU
1	B	615	VAL
1	B	640	ASP
1	B	643	LYS
1	B	645	ASN
1	B	651	PRO
1	B	652	ILE
1	B	656	LEU
1	B	660	ILE
1	B	662	ILE
1	B	663	THR
1	B	670	THR
1	B	672	LEU
1	B	677	LEU
1	B	682	LEU
1	B	685	VAL
1	B	688	ILE
1	B	691	HIS
1	B	699	HIS
1	B	702	ASP
1	B	704	ARG
1	B	708	LEU
1	B	724	ASN
1	B	725	LEU
1	B	741	HIS
1	B	746	TYR
1	B	747	VAL
1	B	748	ASP
1	B	758	ARG
1	B	759	GLU
1	B	777	TYR
1	B	782	GLU
1	B	788	ILE
1	B	797	ILE
1	B	800	LEU
1	B	803	VAL
1	B	811	LEU
1	B	812	LEU

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Mol	Chain	Res	Type
1	B	814	THR
1	B	827	ILE
1	B	828	LEU
1	B	839	MET
1	B	843	LYS
1	B	846	VAL
1	B	852	ILE
1	B	855	GLU
1	B	859	GLU
1	B	863	GLN
1	B	866	THR
1	B	869	LEU
1	B	876	ASN
1	B	881	LEU
1	B	889	THR
1	B	895	LEU
1	B	898	ASP
1	B	914	ASP
1	B	920	HIS
1	B	923	SER
1	B	924	LEU
1	B	940	ILE
1	B	944	THR
1	B	948	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	340	ASN
1	A	356	ASN
1	A	375	HIS
1	A	377	GLN
1	A	403	GLN
1	A	532	ASN
1	A	568	GLN
1	A	573	HIS
1	A	645	ASN
1	A	699	HIS
1	A	764	ASN
1	A	807	HIS
1	A	810	ASN

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Mol	Chain	Res	Type
1	A	876	ASN
1	A	922	GLN
1	B	340	ASN
1	B	349	GLN
1	B	403	GLN
1	B	532	ASN
1	B	549	ASN
1	B	568	GLN
1	B	573	HIS
1	B	589	ASN
1	B	711	GLN
1	B	741	HIS
1	B	745	GLN
1	B	807	HIS
1	B	810	ASN
1	B	857	HIS
1	B	876	ASN
1	B	922	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	090	A	1949	-	27,29,29	4.03	14 (51%)	32,41,41	1.94	7 (21%)
2	090	B	1950	-	27,29,29	4.10	16 (59%)	32,41,41	1.84	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	090	A	1949	-	-	1/12/12/12	0/4/4/4
2	090	B	1950	-	-	1/12/12/12	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1949	090	CAB-CAH	10.89	1.55	1.35
2	B	1950	090	CAB-CAH	10.58	1.54	1.35
2	B	1950	090	CAB-NAA	8.88	1.54	1.38
2	A	1949	090	CAB-NAA	8.25	1.53	1.38
2	B	1950	090	CAM-NAL	7.86	1.46	1.33
2	A	1949	090	CAM-NAL	7.52	1.45	1.33
2	A	1949	090	CAQ-CAP	7.46	1.51	1.39
2	B	1950	090	CAQ-CAP	7.33	1.50	1.39
2	B	1950	090	CAF-NAA	5.14	1.47	1.36
2	A	1949	090	CAJ-CAK	-4.99	1.36	1.42
2	B	1950	090	CAF-CAE	4.76	1.52	1.44
2	A	1949	090	CAF-NAA	4.66	1.46	1.36
2	A	1949	090	CAK-NAL	4.26	1.45	1.37
2	A	1949	090	CAF-CAE	4.02	1.51	1.44
2	B	1950	090	CAO-NAN	3.93	1.47	1.35
2	B	1950	090	CAK-NAL	3.90	1.45	1.37
2	A	1949	090	CAO-NAN	3.57	1.46	1.35
2	B	1950	090	CAJ-CAK	-3.35	1.38	1.42
2	B	1950	090	CAV-CAP	-2.84	1.35	1.39
2	B	1950	090	CAW-CAX	2.83	1.45	1.37
2	A	1949	090	CAW-CAX	2.55	1.45	1.37
2	A	1949	090	OAS-CAI	2.38	1.41	1.37
2	B	1950	090	CAD-CAC	2.32	1.41	1.36
2	A	1949	090	CAV-CAP	-2.31	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1950	090	OAS-CAI	2.28	1.40	1.37
2	B	1950	090	CAX-NAR	2.27	1.40	1.33
2	A	1949	090	CAP-CAO	2.22	1.55	1.50
2	A	1949	090	CAX-NAR	2.20	1.40	1.33
2	B	1950	090	CAD-CAE	-2.12	1.38	1.42
2	B	1950	090	CAC-CAI	2.06	1.43	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1950	090	CAE-CAF-NAA	6.39	135.39	120.88
2	A	1949	090	CAE-CAF-NAA	5.56	133.51	120.88
2	A	1949	090	OAS-CAI-CAJ	3.77	120.96	116.44
2	B	1950	090	CAB-CAH-NAG	-3.65	102.27	106.87
2	A	1949	090	CAY-OAS-CAI	3.55	122.72	117.51
2	A	1949	090	CAD-CAE-CAF	-3.42	119.04	123.49
2	A	1949	090	OAS-CAI-CAC	-3.40	118.56	124.30
2	B	1950	090	CAJ-CAK-CAE	2.92	122.14	119.29
2	A	1949	090	CAF-CAE-CAK	2.76	119.91	117.17
2	A	1949	090	CAB-CAH-NAG	-2.50	103.72	106.87
2	B	1950	090	CAV-CAP-CAQ	2.45	120.34	117.61
2	B	1950	090	CAF-CAE-CAK	2.38	119.53	117.17
2	B	1950	090	CAZ-OAT-CAJ	2.29	121.06	114.88
2	B	1950	090	CAY-OAS-CAI	2.02	120.47	117.51

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1949	090	OAU-CAO-NAN-CAM
2	B	1950	090	CAP-CAO-NAN-CAM

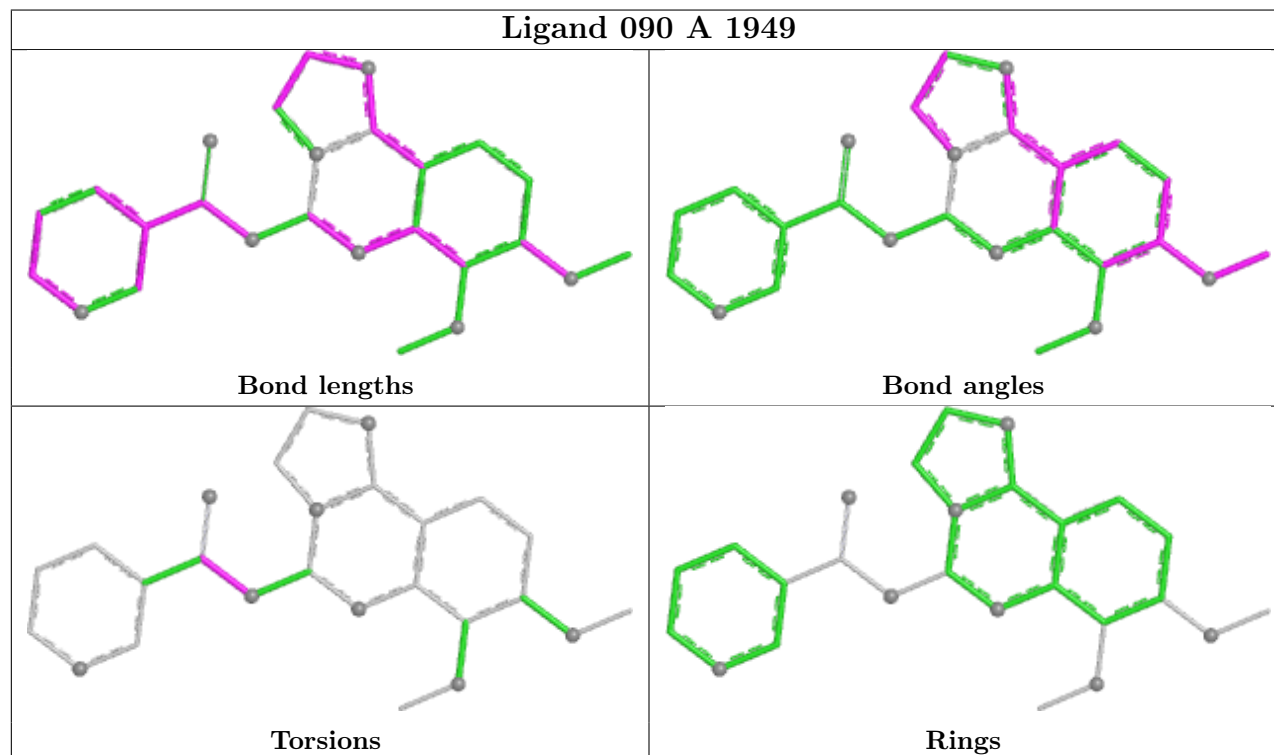
There are no ring outliers.

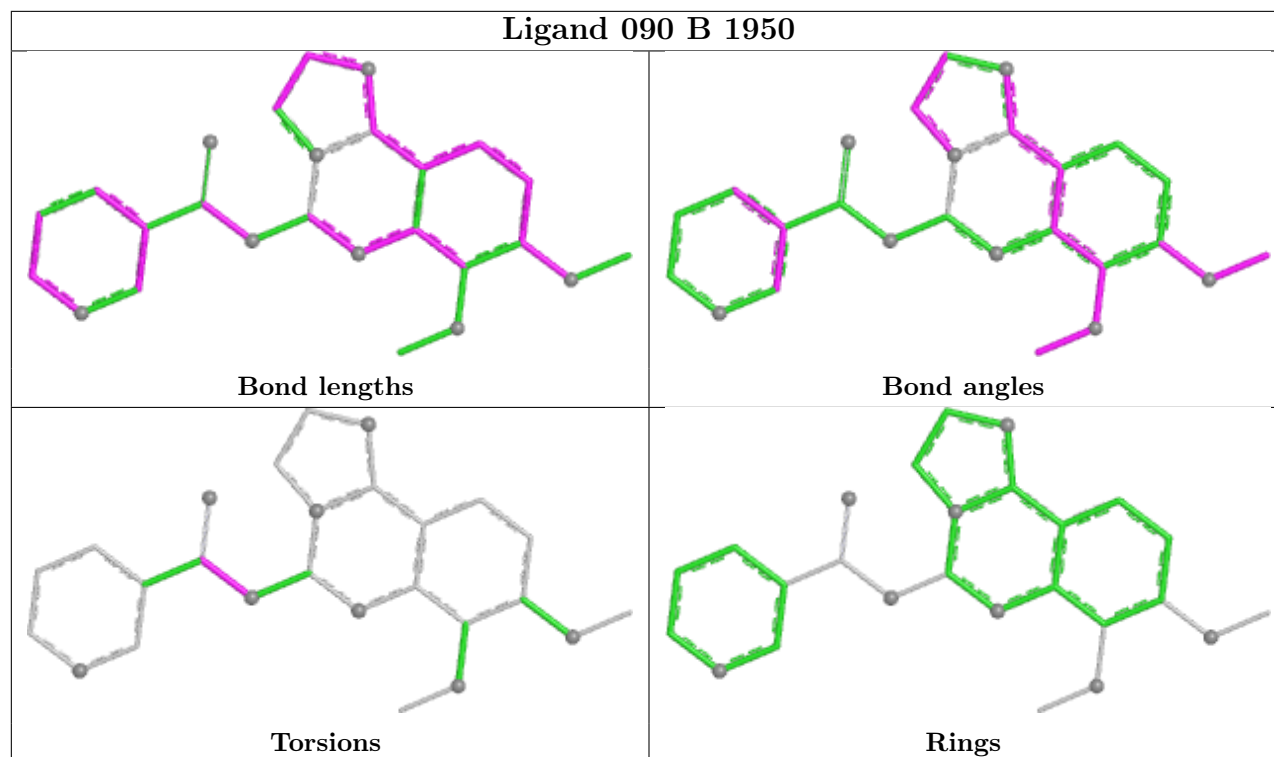
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1949	090	3	0
2	B	1950	090	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	546/696 (78%)	0.11	12 (2%) 62 47	36, 59, 97, 114	0
1	B	544/696 (78%)	-0.08	6 (1%) 78 65	47, 70, 100, 110	0
All	All	1090/1392 (78%)	0.02	18 (1%) 69 54	36, 65, 99, 114	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	302	TYR	7.9
1	B	302	TYR	4.7
1	B	340	ASN	3.9
1	A	293	ILE	3.2
1	A	305	PRO	3.0
1	A	348	THR	2.9
1	A	351	LEU	2.8
1	B	293	ILE	2.7
1	B	310	LEU	2.6
1	A	339	ILE	2.6
1	A	590	GLY	2.5
1	A	325	LEU	2.4
1	B	319	TRP	2.4
1	A	310	LEU	2.3
1	A	324	TYR	2.2
1	A	322	ARG	2.2
1	B	306	PRO	2.1
1	A	323	PHE	2.1

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](#)

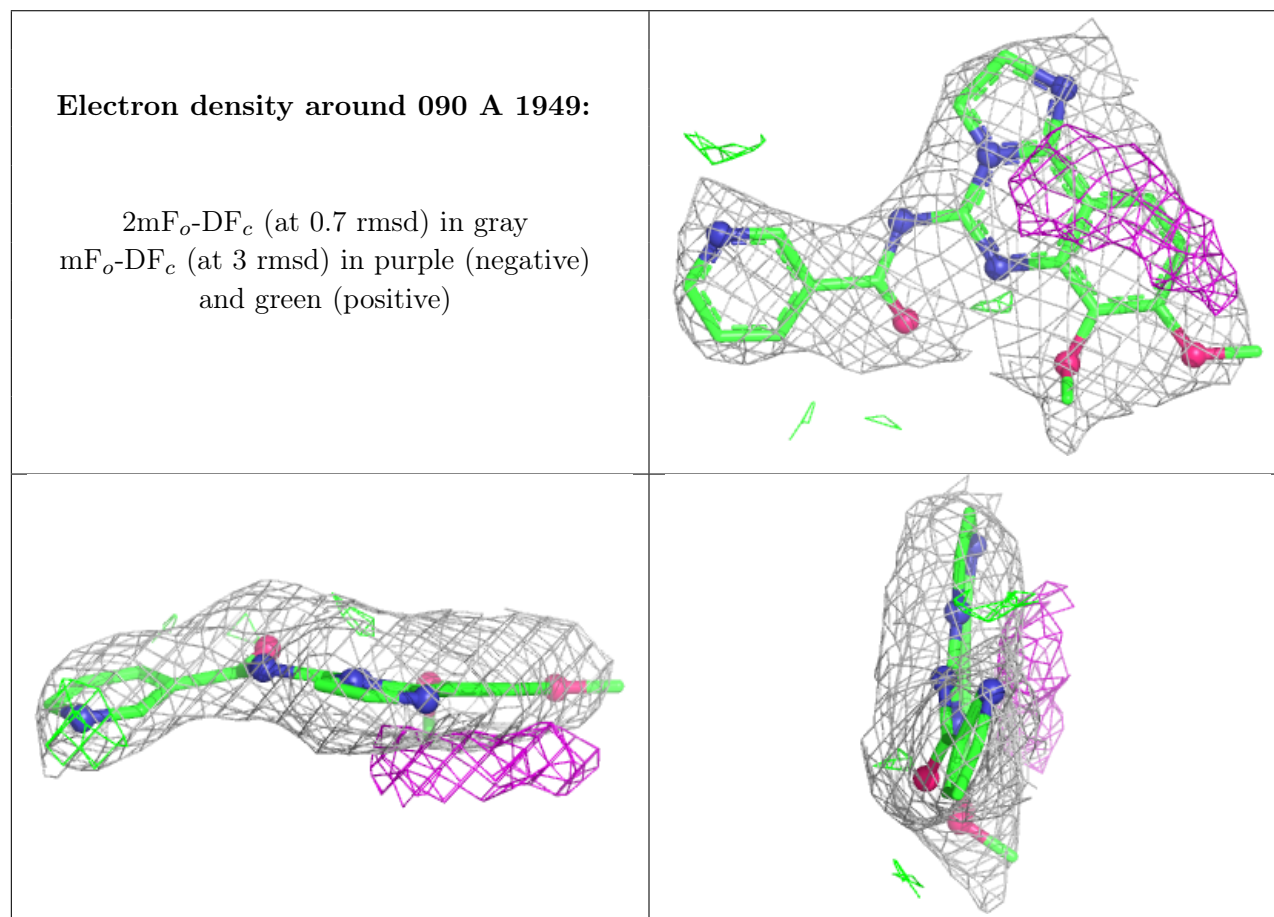
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

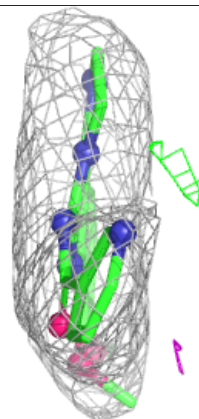
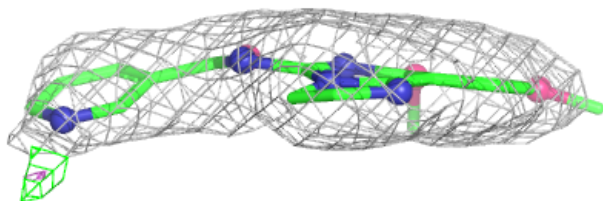
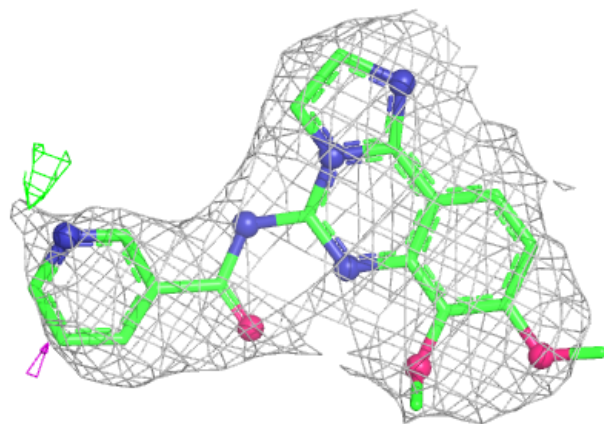
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	090	A	1949	26/26	0.90	0.15	69,77,87,88	0
2	090	B	1950	26/26	0.94	0.11	75,80,95,96	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around 090 B 1950:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.