



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:00 PM UTC

PDB ID : 5URM / pdb_00005urm
Title : Crystal structure of human BRR2 in complex with T-1206548
Authors : Klein, M.G.; Tjhen, R.; Qin, L.
Deposited on : 2017-02-11
Resolution : 2.80 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

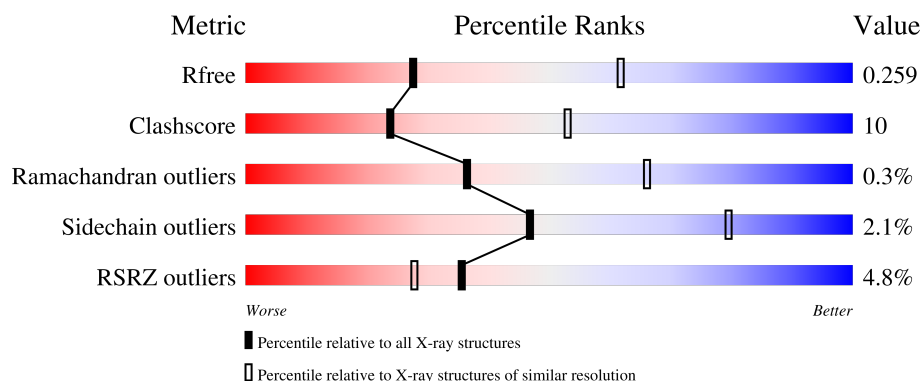
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	1738	5% 73% 24% ..
1	B	1738	5% 71% 25% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 27571 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.

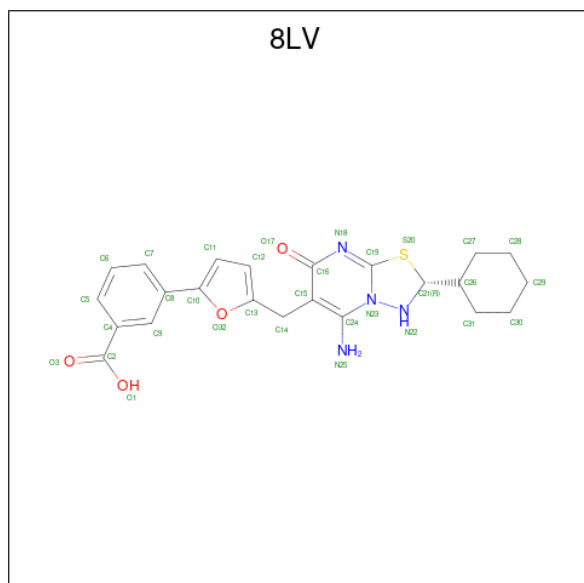
- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1718	Total	C	N	O	S	0	0	0
			13802	8821	2360	2550	71			
1	B	1691	Total	C	N	O	S	0	0	0
			13603	8705	2323	2504	71			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	GLY	-	expression tag	UNP O75643
A	393	GLY	-	expression tag	UNP O75643
A	394	SER	-	expression tag	UNP O75643
B	392	GLY	-	expression tag	UNP O75643
B	393	GLY	-	expression tag	UNP O75643
B	394	SER	-	expression tag	UNP O75643

- Molecule 2 is 3-(5-{[(2R)-5-amino-2-cyclohexyl-7-oxo-2,3-dihydro-7H-[1,3,4]thiadiazolo[3,2-a]pyrimidin-6-yl]methyl}furan-2-yl)benzoic acid (CCD ID: 8LV) (formula: C₂₃H₂₄N₄O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	23	4	4	1		
2	B	1	Total	C	N	O	S	0	0
			32	23	4	4	1		

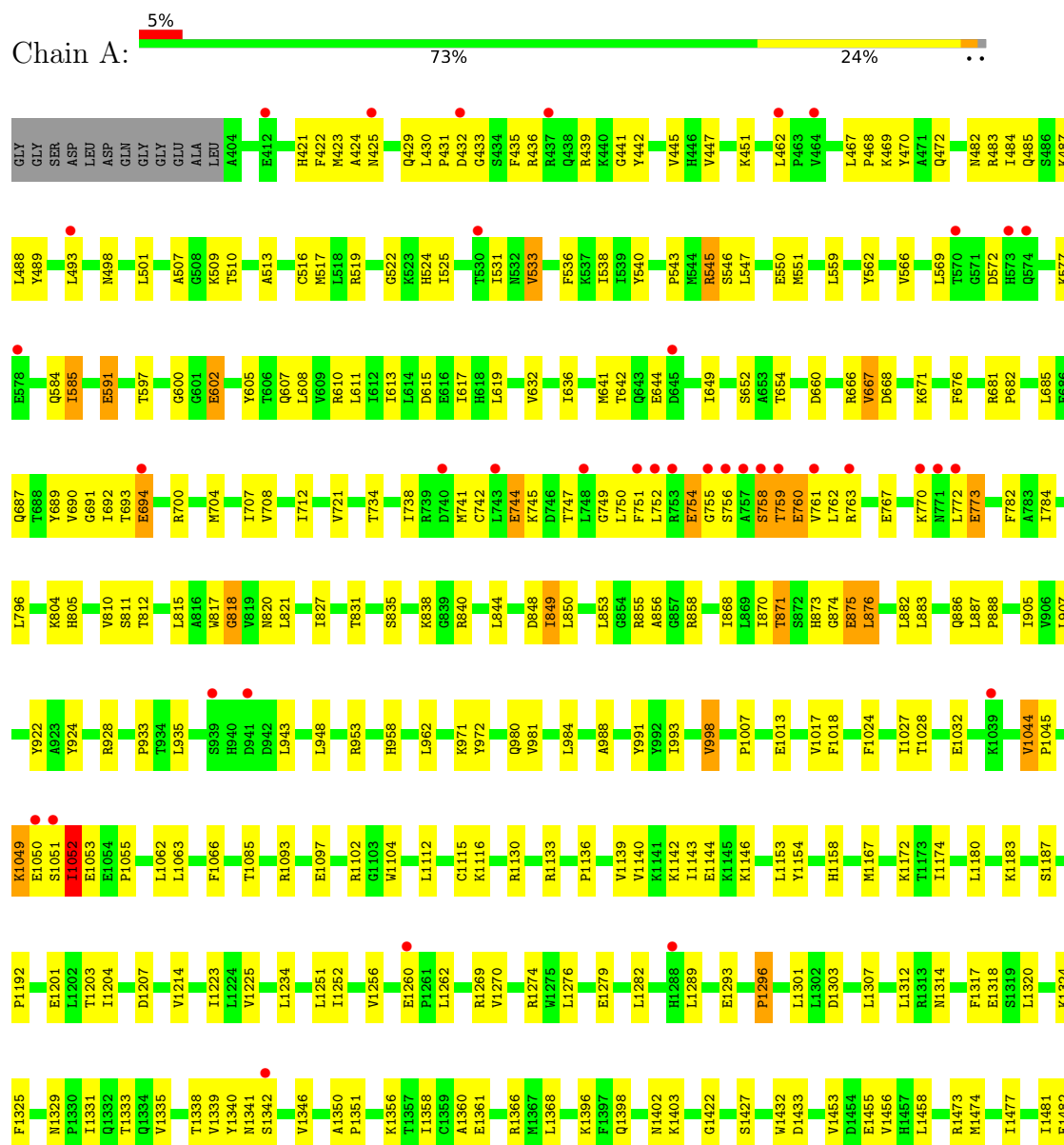
- Molecule 3 is water.

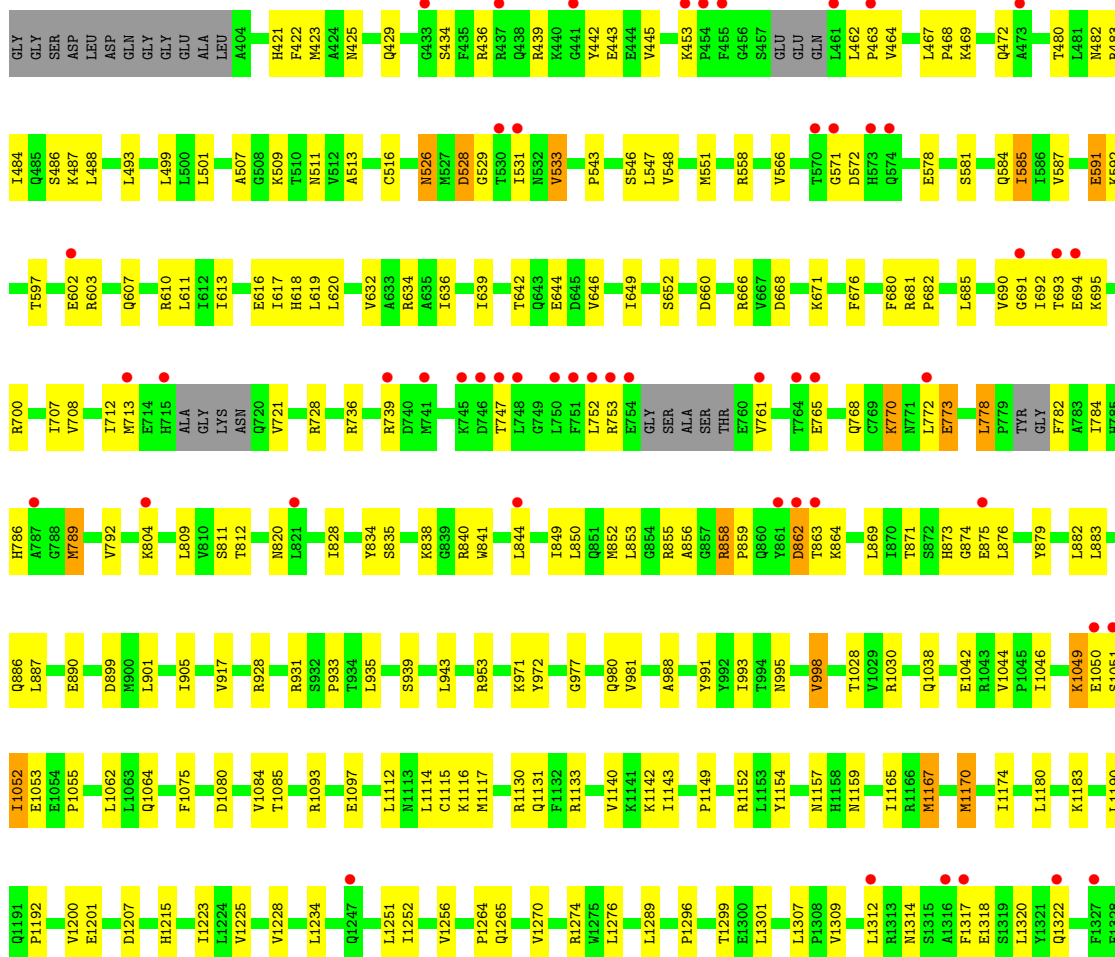
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	44	Total	O	0	0
			44	44		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: U5 small nuclear ribonucleoprotein 200 kDa helicase







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.86Å 105.87Å 135.28Å 71.14° 70.48° 89.83°	Depositor
Resolution (Å)	29.48 – 2.80 29.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.48-2.80) 98.1 (29.48-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.260 0.215 , 0.259	Depositor DCC
R_{free} test set	6206 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27571	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8LV

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	0.41	0/14095	0.90	33/19100 (0.2%)
1	B	0.41	0/13889	0.89	28/18815 (0.1%)
All	All	0.41	0/27984	0.90	61/37915 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	7
All	All	0	13

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	GLY	N-CA-C	-12.22	89.98	111.62
1	A	874	GLY	N-CA-C	-9.38	101.14	111.93
1	A	1987	GLU	N-CA-C	-9.30	100.88	112.88
1	B	874	GLY	N-CA-C	-8.90	101.69	111.93
1	A	1422	GLY	N-CA-C	8.70	123.20	111.03
1	B	858	ARG	CA-C-N	8.00	127.29	118.97
1	B	858	ARG	C-N-CA	8.00	127.29	118.97
1	B	2056	PHE	CA-C-N	7.96	127.62	119.19
1	B	2056	PHE	C-N-CA	7.96	127.62	119.19
1	B	862	ASP	N-CA-C	7.79	122.30	109.06
1	A	744	GLU	N-CA-C	7.77	119.50	108.00
1	A	1044	VAL	CA-C-N	7.76	127.31	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1044	VAL	C-N-CA	7.76	127.31	118.85
1	A	751	PHE	N-CA-C	-7.75	103.64	113.72
1	A	447	VAL	CA-C-N	7.54	127.49	120.03
1	A	447	VAL	C-N-CA	7.54	127.49	120.03
1	B	1993	ARG	N-CA-C	7.33	120.20	111.33
1	B	835	SER	CA-C-N	7.26	127.11	119.05
1	B	835	SER	C-N-CA	7.26	127.11	119.05
1	B	1422	GLY	N-CA-C	6.79	120.53	111.03
1	A	1732	MET	N-CA-C	6.77	120.41	111.75
1	A	2043	ARG	N-CA-C	6.73	120.14	109.50
1	A	744	GLU	CB-CA-C	-6.66	107.01	116.34
1	A	451	LYS	CA-C-N	6.61	128.10	119.84
1	A	451	LYS	C-N-CA	6.61	128.10	119.84
1	B	526	ASN	N-CA-C	6.58	120.16	111.28
1	A	835	SER	CA-C-N	6.25	125.99	119.05
1	A	835	SER	C-N-CA	6.25	125.99	119.05
1	B	747	THR	CA-C-N	-6.12	113.78	122.41
1	B	747	THR	C-N-CA	-6.12	113.78	122.41
1	A	747	THR	N-CA-C	6.11	119.22	110.24
1	B	789	MET	CB-CA-C	-6.09	107.85	115.89
1	B	1044	VAL	CA-C-N	6.01	125.40	118.85
1	B	1044	VAL	C-N-CA	6.01	125.40	118.85
1	A	2047	VAL	N-CA-C	5.78	116.53	108.89
1	A	754	GLU	N-CA-C	-5.65	105.97	112.92
1	B	1598	ILE	CB-CA-C	-5.57	108.41	113.70
1	B	1519	ARG	CA-C-N	5.49	124.95	119.24
1	B	1519	ARG	C-N-CA	5.49	124.95	119.24
1	B	713	MET	N-CA-C	5.44	117.64	111.11
1	A	2017	ILE	N-CA-C	5.41	115.49	108.35
1	B	1167	MET	CA-C-N	5.37	125.04	119.56
1	B	1167	MET	C-N-CA	5.37	125.04	119.56
1	B	453	LYS	N-CA-C	5.33	116.12	109.57
1	A	435	PHE	N-CA-C	5.31	117.15	109.07
1	B	721	VAL	N-CA-C	5.28	115.51	108.11
1	B	695	LYS	N-CA-C	5.26	118.00	109.79
1	A	1991	GLU	N-CA-C	5.25	121.99	110.80
1	A	694	GLU	N-CA-C	5.19	116.55	109.18
1	A	1282	LEU	CA-C-N	-5.19	114.57	119.76
1	A	1282	LEU	C-N-CA	-5.19	114.57	119.76
1	A	1427	SER	N-CA-C	5.18	116.94	109.07
1	A	1990	ASP	N-CA-C	-5.16	99.81	110.80
1	A	1052	ILE	CA-C-N	-5.13	113.28	122.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1052	ILE	C-N-CA	-5.13	113.28	122.32
1	A	424	ALA	N-CA-C	-5.10	106.56	112.89
1	A	818	GLY	N-CA-C	5.09	120.20	113.37
1	A	1296	PRO	CA-C-N	5.03	123.33	119.66
1	A	1296	PRO	C-N-CA	5.03	123.33	119.66
1	B	1052	ILE	CA-C-N	-5.02	113.49	122.32
1	B	1052	ILE	C-N-CA	-5.02	113.49	122.32

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1049	LYS	Peptide
1	A	1988	MET	Peptide
1	A	1989	GLU	Peptide
1	A	2058	GLN	Peptide
1	A	694	GLU	Peptide
1	A	758	SER	Peptide
1	B	1049	LYS	Peptide
1	B	1482	GLU	Peptide
1	B	1988	MET	Peptide
1	B	2058	GLN	Peptide
1	B	528	ASP	Peptide
1	B	694	GLU	Peptide
1	B	862	ASP	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	13802	0	13922	293	0
1	B	13603	0	13739	275	0
2	A	32	0	0	3	0
2	B	32	0	0	2	0
3	A	58	0	0	0	0
3	B	44	0	0	2	0
All	All	27571	0	27661	557	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 10.

All (557) 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:B:2040:GLN:NE2	1:B:2088:ALA:O	1.99	0.95
1:A:742:CYS:HB3	1:A:749:GLY:HA2	1.53	0.89
1:B:572:ASP:OD1	1:B:1274:ARG:NH1	2.09	0.83
1:A:666:ARG:HH11	1:B:1595:LYS:HD3	1.44	0.82
1:A:421:HIS:NE2	1:A:875:GLU:OE2	2.15	0.79
1:B:1587:GLN:NE2	1:B:1594:GLU:OE2	2.16	0.79
1:A:1594:GLU:HG3	1:A:1614:LEU:HD22	1.65	0.78
1:B:1819:ALA:HB2	1:B:1829:ILE:HG12	1.65	0.78
1:A:755:GLY:O	1:A:759:THR:OG1	2.01	0.77
1:B:768:GLN:HA	1:B:770:LYS:HE2	1.67	0.76
1:A:1293:GLU:OE1	1:A:1766:GLN:NE2	2.17	0.75
1:B:770:LYS:HE3	1:B:778:LEU:HD13	1.68	0.75
1:A:772:LEU:HG	1:A:773:GLU:H	1.52	0.74
1:B:660:ASP:OD2	1:B:931:ARG:NH1	2.19	0.74
1:B:1375:ARG:NH1	1:B:1419:LEU:O	2.21	0.74
1:A:2029:ILE:HG21	1:A:2035:VAL:HG22	1.70	0.73
1:A:1456:VAL:HG22	1:A:1491:SER:HB2	1.69	0.73
1:A:1351:PRO:HG3	1:A:1516:PRO:HA	1.71	0.73
1:B:736:ARG:HG2	1:B:739:ARG:HH12	1.52	0.73
1:A:2023:VAL:HG22	1:A:2026:LYS:HD2	1.70	0.72
1:B:1130:ARG:HG3	1:B:1140:VAL:HG11	1.72	0.72
1:A:770:LYS:HG2	1:A:796:LEU:HD22	1.72	0.72
1:B:1456:VAL:HG22	1:B:1491:SER:HB2	1.72	0.71
1:A:1989:GLU:HB2	1:A:1991:GLU:HB2	1.73	0.71
1:B:1986:MET:HG3	1:B:2011:CYS:HB3	1.72	0.71
1:A:758:SER:HA	1:A:761:VAL:HB	1.71	0.71
1:B:772:LEU:HG	1:B:773:GLU:H	1.56	0.70
1:A:547:LEU:HD11	1:A:551:MET:HE2	1.73	0.70
1:B:2076:LEU:HD21	1:B:2079:ILE:HB	1.74	0.70
1:B:509:LYS:NZ	1:B:616:GLU:OE1	2.25	0.69
1:B:1350:ALA:HB3	1:B:1356:LYS:HD3	1.74	0.69
1:A:689:TYR:HB3	1:A:876:LEU:HD11	1.74	0.69
1:A:1130:ARG:HG3	1:A:1140:VAL:HG11	1.74	0.69
1:A:988:ALA:HB2	1:A:998:VAL:HG21	1.74	0.69
1:A:666:ARG:HE	1:B:1595:LYS:NZ	1.89	0.69
1:A:1143:ILE:HD11	1:A:1174:ILE:HD13	1.75	0.68
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:HIS:NE2	1:B:875:GLU:OE2	2.27	0.68
1:A:756:SER:HA	1:A:761:VAL:HG21	1.74	0.68
1:B:1358:ILE:HA	1:B:1361:GLU:HB2	1.75	0.67
1:A:708:VAL:O	1:A:712:ILE:HG12	1.95	0.67
1:A:1595:LYS:NZ	1:B:666:ARG:HE	1.92	0.67
1:A:681:ARG:NH2	1:A:856:ALA:O	2.28	0.67
1:A:758:SER:HB2	1:A:762:LEU:HG	1.77	0.67
1:B:772:LEU:HG	1:B:773:GLU:HG3	1.77	0.67
1:B:1991:GLU:HB3	1:B:1993:ARG:HG2	1.75	0.66
1:A:1187:SER:HB3	1:A:1203:THR:HB	1.76	0.66
1:B:1814:ASN:HA	1:B:1817:MET:HE2	1.76	0.66
1:B:690:VAL:HG11	1:B:707:ILE:HD13	1.75	0.66
1:B:841:TRP:HE1	1:B:1030:ARG:HH12	1.42	0.66
1:B:1375:ARG:HG2	1:B:1448:ILE:HG22	1.77	0.66
1:A:1296:PRO:HG3	1:A:1498:LYS:HE2	1.78	0.65
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.78	0.65
1:B:469:LYS:H	1:B:469:LYS:HD2	1.62	0.65
1:B:591:GLU:HG3	2:B:2501:SLV:C8	2.27	0.65
1:B:988:ALA:HB2	1:B:998:VAL:HG21	1.78	0.64
1:B:1049:LYS:O	1:B:1051:SER:N	2.31	0.64
1:B:1585:GLN:HG2	1:B:1588:ARG:HB2	1.79	0.64
1:A:1595:LYS:HD3	1:B:666:ARG:HH11	1.61	0.64
1:B:1143:ILE:HD11	1:B:1174:ILE:HD13	1.79	0.64
1:A:1992:GLU:HB2	1:A:1995:ALA:HB3	1.81	0.63
1:A:1130:ARG:O	1:A:1133:ARG:NH1	2.31	0.63
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.81	0.63
1:B:1028:THR:HA	1:B:1055:PRO:HG3	1.80	0.63
1:A:1049:LYS:O	1:A:1051:SER:N	2.32	0.62
1:A:1320:LEU:HD13	1:A:1396:LYS:HG2	1.80	0.62
1:A:488:LEU:HD11	1:A:501:LEU:HD13	1.81	0.62
1:A:704:MET:HG3	1:A:870:ILE:HG21	1.80	0.62
1:A:820:ASN:OD1	1:A:855:ARG:NH1	2.33	0.62
1:A:2054:PRO:HG2	1:A:2055:LEU:HD12	1.80	0.62
1:A:666:ARG:HE	1:B:1595:LYS:HZ2	1.47	0.62
1:B:1375:ARG:HH12	1:B:1444:ASN:HB3	1.64	0.62
1:B:1560:ILE:HD11	1:B:1656:VAL:HG12	1.82	0.62
1:A:1368:LEU:HD22	1:A:1403:LYS:HE2	1.81	0.61
1:B:603:ARG:O	1:B:607:GLN:HB2	1.99	0.61
1:B:2067:VAL:HG22	1:B:2079:ILE:HG13	1.81	0.61
1:A:815:LEU:HD11	1:A:821:LEU:HD21	1.81	0.61
1:B:482:ASN:OD1	1:B:483:ARG:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:LEU:HD13	1:A:1214:VAL:HG21	1.83	0.61
1:A:538:ILE:HB	1:A:585:ILE:HG13	1.83	0.61
1:A:2040:GLN:NE2	1:A:2088:ALA:O	2.34	0.61
1:B:1711:LYS:HG2	1:B:1715:LYS:HE2	1.81	0.60
1:A:1028:THR:HA	1:A:1055:PRO:HG3	1.83	0.60
1:B:484:ILE:HD12	1:B:507:ALA:HB1	1.82	0.60
1:B:543:PRO:HB3	1:B:619:LEU:HD22	1.84	0.60
1:B:2054:PRO:HG2	1:B:2055:LEU:HD12	1.84	0.60
1:B:692:ILE:HG21	1:B:700:ARG:HG3	1.83	0.60
1:A:1142:LYS:HE3	1:A:1146:LYS:HZ3	1.67	0.60
1:A:1358:ILE:HA	1:A:1361:GLU:HB2	1.83	0.60
1:A:517:MET:HE3	1:A:585:ILE:HG12	1.85	0.59
1:B:1748:LYS:NZ	1:B:1790:GLU:OE2	2.27	0.59
1:B:488:LEU:HD11	1:B:501:LEU:HD13	1.84	0.59
1:A:2084:LEU:HD12	1:A:2085:GLN:H	1.67	0.59
1:A:1482:GLU:HG2	1:A:1483:ARG:H	1.67	0.58
1:A:692:ILE:HG21	1:A:700:ARG:HG3	1.84	0.58
1:A:1593:THR:HG22	1:A:1595:LYS:H	1.68	0.58
1:B:2013:ARG:HD3	1:B:2050:PRO:O	2.03	0.58
1:B:849:ILE:HG22	1:B:883:LEU:HD21	1.84	0.58
1:A:1883:LYS:HG3	1:A:1886:ASP:HB2	1.86	0.58
1:A:1142:LYS:HE3	1:A:1146:LYS:NZ	2.18	0.58
1:B:566:VAL:HG22	1:B:585:ILE:HB	1.84	0.58
1:A:971:LYS:HB2	1:A:980:GLN:HB2	1.87	0.57
1:B:1341:ASN:O	1:B:1366:ARG:NH1	2.36	0.57
1:A:566:VAL:HG22	1:A:585:ILE:HB	1.86	0.57
1:A:666:ARG:NH1	1:B:1595:LYS:HD3	2.18	0.57
1:B:1993:ARG:HG3	1:B:1994:ASN:N	2.19	0.57
1:B:2003:GLN:HA	1:B:2006:ASP:HB2	1.87	0.57
1:A:1350:ALA:HB3	1:A:1356:LYS:HD3	1.87	0.57
1:B:1192:PRO:HG3	1:B:1289:LEU:HD11	1.87	0.57
1:A:1130:ARG:NE	1:A:1144:GLU:OE2	2.38	0.57
1:A:1192:PRO:HG3	1:A:1289:LEU:HD11	1.86	0.57
1:A:804:LYS:HE3	1:A:858:ARG:HH12	1.68	0.57
1:B:708:VAL:O	1:B:712:ILE:HG12	2.05	0.56
1:A:1963:LEU:HD22	1:A:2007:VAL:HG13	1.86	0.56
1:A:611:LEU:HD11	1:A:649:ILE:HD13	1.86	0.56
1:B:1883:LYS:HG3	1:B:1886:ASP:HB2	1.85	0.56
1:A:572:ASP:OD1	1:A:1274:ARG:NH1	2.39	0.56
1:A:2030:ARG:HG2	1:A:2031:SER:H	1.69	0.56
1:B:468:PRO:HD2	1:B:493:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1360:ALA:HB2	1:A:1490:LEU:HD11	1.87	0.56
1:A:1883:LYS:HE2	1:A:1886:ASP:HB2	1.87	0.56
1:B:811:SER:OG	1:B:812:THR:N	2.39	0.56
1:B:1962:GLN:NE2	1:B:2114:MET:O	2.35	0.56
1:A:1661:VAL:HG23	1:A:1691:ALA:HB2	1.88	0.56
1:A:1112:LEU:HG	1:A:1116:LYS:HE3	1.88	0.55
1:A:2084:LEU:HD12	1:A:2085:GLN:N	2.22	0.55
1:B:681:ARG:HG3	1:B:682:PRO:HD2	1.89	0.55
1:A:817:TRP:NE1	1:A:848:ASP:OD1	2.35	0.55
1:B:513:ALA:HB1	1:B:613:ILE:HD13	1.88	0.55
1:A:2069:GLY:HA2	1:A:2077:ILE:HG12	1.88	0.55
1:B:571:GLY:HA2	1:B:592:LYS:NZ	2.22	0.55
1:A:1819:ALA:HB2	1:A:1829:ILE:HG12	1.87	0.55
1:A:2017:ILE:HA	1:A:2043:ARG:CZ	2.37	0.55
1:B:752:LEU:HD13	1:B:782:PHE:HE1	1.70	0.55
1:A:1585:GLN:HG2	1:A:1588:ARG:HB2	1.88	0.55
1:A:1595:LYS:HZ3	1:B:666:ARG:HE	1.55	0.55
1:B:429:GLN:O	1:B:886:GLN:NE2	2.40	0.55
1:A:2017:ILE:HG21	1:A:2108:PHE:HE2	1.72	0.55
1:B:1815:LEU:HB3	1:B:1829:ILE:HD13	1.88	0.55
1:B:820:ASN:OD1	1:B:855:ARG:NH1	2.40	0.55
1:B:863:THR:HG22	1:B:864:LYS:H	1.70	0.55
1:A:2076:LEU:HD21	1:A:2079:ILE:HB	1.89	0.54
1:B:2000:THR:O	1:B:2004:ILE:HG12	2.07	0.54
1:A:2018:GLU:H	1:A:2043:ARG:NH2	2.06	0.54
1:A:2019:LEU:HD13	1:A:2041:LEU:HD23	1.89	0.54
1:B:1434:ILE:HD13	1:B:1823:TYR:HB2	1.88	0.54
1:A:484:ILE:HD12	1:A:507:ALA:HB1	1.89	0.54
1:A:1553:HIS:O	1:A:1701:ARG:NH1	2.36	0.54
1:A:1482:GLU:HG2	1:A:1483:ARG:N	2.23	0.54
1:B:423:MET:HE2	1:B:425:ASN:HB3	1.90	0.54
1:B:1661:VAL:HG23	1:B:1691:ALA:HB2	1.88	0.54
1:B:1964:PRO:HB2	1:B:1965:HIS:ND1	2.23	0.54
1:A:467:LEU:HB2	1:A:468:PRO:HD2	1.89	0.54
1:A:2043:ARG:HD3	1:A:2044:GLU:H	1.72	0.54
1:A:2017:ILE:HG22	1:A:2118:GLN:HE22	1.73	0.54
1:B:2038:LEU:HD12	1:B:2091:LYS:HG2	1.90	0.53
1:A:827:ILE:HG12	1:A:868:ILE:HD13	1.90	0.53
1:B:804:LYS:HD2	1:B:804:LYS:N	2.23	0.53
1:A:1711:LYS:HG2	1:A:1715:LYS:HD2	1.91	0.53
1:B:1566:ARG:HG3	1:B:1621:HIS:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1988:MET:SD	1:B:1992:GLU:HG2	2.49	0.53
1:A:524:HIS:CE1	1:A:536:PHE:HB3	2.44	0.53
1:A:905:ILE:HG22	1:A:981:VAL:HG22	1.91	0.53
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	1.90	0.53
1:A:958:HIS:ND1	1:A:972:TYR:OH	2.39	0.52
1:A:577:LYS:HE2	1:A:605:TYR:OH	2.10	0.52
1:A:811:SER:OG	1:A:812:THR:N	2.42	0.52
1:A:1901:ARG:HD2	1:A:1961:LYS:HE2	1.91	0.52
1:B:1117:MET:HG2	1:B:1276:LEU:HD11	1.91	0.52
1:B:1375:ARG:HB3	1:B:1448:ILE:HA	1.91	0.52
1:A:754:GLU:C	1:A:756:SER:H	2.17	0.52
1:A:2017:ILE:HD13	1:A:2108:PHE:HE2	1.74	0.52
1:A:436:ARG:HG2	1:A:445:VAL:HG22	1.90	0.52
1:A:1312:LEU:HD12	1:A:1340:TYR:CZ	2.45	0.52
1:B:1855:TYR:HB3	1:B:1891:THR:HG21	1.92	0.52
1:A:617:ILE:HG22	1:A:652:SER:HB2	1.92	0.52
1:A:1814:ASN:HA	1:A:1817:MET:HE2	1.91	0.52
1:A:1970:HIS:CG	1:A:1971:ILE:H	2.27	0.52
1:B:765:GLU:O	1:B:768:GLN:HG2	2.10	0.52
1:B:1335:VAL:O	1:B:1339:VAL:HG12	2.10	0.52
1:A:691:GLY:HA2	1:A:871:THR:O	2.09	0.52
1:A:591:GLU:HG3	2:A:2501:8LV:C8	2.40	0.52
1:A:2017:ILE:HG22	1:A:2118:GLN:NE2	2.24	0.52
1:B:736:ARG:HG2	1:B:739:ARG:NH1	2.24	0.52
1:B:786:HIS:CD2	1:B:789:MET:HE3	2.45	0.52
1:A:1346:VAL:HG13	1:A:1488:VAL:HG13	1.92	0.51
1:B:691:GLY:HA2	1:B:871:THR:O	2.09	0.51
1:A:516:CYS:SG	1:A:649:ILE:HG12	2.50	0.51
1:B:1398:GLN:O	1:B:1402:ASN:HA	2.10	0.51
1:A:482:ASN:HB3	1:A:485:GLN:CD	2.36	0.51
1:A:513:ALA:HB1	1:A:613:ILE:HD13	1.92	0.51
1:A:1225:VAL:HG11	1:A:1256:VAL:HG11	1.93	0.51
1:B:668:ASP:HB3	1:B:671:LYS:HB2	1.93	0.51
1:B:1165:ILE:HG13	1:B:1167:MET:H	1.74	0.51
1:B:617:ILE:HG22	1:B:652:SER:HB2	1.93	0.51
1:B:597:THR:OG1	1:B:634:ARG:NH1	2.43	0.51
1:B:1329:ASN:O	1:B:1333:THR:HG23	2.10	0.51
1:B:1948:MET:HB2	1:B:1953:MET:O	2.10	0.51
1:A:498:ASN:HB3	1:A:667:VAL:HG12	1.93	0.51
1:A:804:LYS:HE3	1:A:858:ARG:NH1	2.26	0.51
1:B:2069:GLY:HA2	1:B:2077:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1815:LEU:HB3	1:A:1829:ILE:HD13	1.93	0.51
1:A:1987:GLU:O	1:A:1988:MET:HG2	2.10	0.51
1:B:2103:ASN:OD1	1:B:2123:SER:OG	2.28	0.51
1:A:522:GLY:O	1:A:525:ILE:HG13	2.11	0.51
1:A:525:ILE:HA	1:A:531:ILE:HD12	1.92	0.51
1:A:831:THR:OG1	1:A:871:THR:HG23	2.10	0.50
1:A:1528:GLN:HG2	1:A:1530:PHE:CE2	2.46	0.50
1:A:1560:ILE:HD11	1:A:1656:VAL:HG12	1.93	0.50
1:B:487:LYS:HD3	1:B:676:PHE:CE2	2.47	0.50
1:B:1296:PRO:HG3	1:B:1498:LYS:HD3	1.93	0.50
1:A:493:LEU:O	1:A:519:ARG:HD2	2.11	0.50
1:B:1170:MET:HE3	1:B:1170:MET:HA	1.92	0.50
1:A:984:LEU:HD21	1:A:1102:ARG:HH21	1.77	0.50
1:A:1024:PHE:HB3	1:A:1027:ILE:HD12	1.92	0.50
1:A:2000:THR:O	1:A:2004:ILE:HG12	2.12	0.50
1:B:890:GLU:CD	1:B:928:ARG:HH21	2.20	0.50
1:A:988:ALA:HA	1:A:993:ILE:HG12	1.93	0.49
1:B:1745:ILE:HA	1:B:1750:ASP:HB3	1.94	0.49
1:A:550:GLU:HB2	1:A:818:GLY:O	2.12	0.49
1:B:828:ILE:HD13	1:B:852:MET:HE3	1.94	0.49
1:B:863:THR:HG22	1:B:864:LYS:N	2.27	0.49
1:B:2109:MET:HE2	1:B:2117:ASP:OD2	2.13	0.49
1:A:1314:ASN:O	1:A:1318:GLU:HG3	2.13	0.49
1:B:1183:LYS:HB3	1:B:1207:ASP:O	2.12	0.49
1:A:1154:TYR:CE1	1:A:1183:LYS:HD2	2.48	0.49
1:B:463:PRO:HA	1:B:480:THR:HA	1.93	0.49
1:A:1093:ARG:HD2	1:A:1115:CYS:SG	2.53	0.49
1:A:2016:ASN:O	1:A:2017:ILE:HG13	2.12	0.49
1:B:1053:GLU:N	1:B:1053:GLU:OE1	2.46	0.49
1:B:850:LEU:HD23	1:B:883:LEU:HD23	1.94	0.49
1:A:1341:ASN:O	1:A:1366:ARG:NH1	2.46	0.49
1:B:2016:ASN:O	1:B:2043:ARG:HG3	2.13	0.49
1:A:873:HIS:O	1:A:876:LEU:HB2	2.12	0.48
1:B:991:TYR:CE1	1:B:1097:GLU:HG3	2.48	0.48
1:A:1335:VAL:O	1:A:1339:VAL:HG12	2.14	0.48
1:A:1453:VAL:HG22	1:A:1456:VAL:HG12	1.94	0.48
1:B:1228:VAL:HG21	1:B:1264:PRO:HD2	1.96	0.48
1:A:482:ASN:OD1	1:A:483:ARG:N	2.46	0.48
1:A:1741:VAL:HG13	1:A:1817:MET:HG2	1.95	0.48
1:B:784:ILE:O	1:B:789:MET:HE1	2.13	0.48
1:B:933:PRO:HG3	1:B:943:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1309:VAL:HB	1:B:1322:GLN:NE2	2.28	0.48
1:A:429:GLN:H	1:A:886:GLN:HE22	1.60	0.48
1:A:2017:ILE:HG21	1:A:2108:PHE:CE2	2.49	0.48
1:B:422:PHE:HZ	1:B:935:LEU:HD11	1.78	0.48
1:B:1515:HIS:O	1:B:1518:VAL:HG22	2.13	0.48
1:B:1345:ASN:OD1	1:B:1487:ILE:N	2.39	0.48
1:B:972:TYR:HE2	1:B:977:GLY:HA2	1.78	0.48
1:A:668:ASP:HB3	1:A:671:LYS:HB2	1.96	0.48
1:A:1855:TYR:HA	1:A:1858:ILE:HD13	1.95	0.48
1:B:1038:GLN:O	1:B:1042:GLU:HG2	2.14	0.48
1:A:2067:VAL:HG22	1:A:2079:ILE:HG13	1.95	0.48
1:B:1190:LEU:HD23	1:B:1200:VAL:HG22	1.96	0.48
1:B:436:ARG:HG2	1:B:445:VAL:HG22	1.96	0.47
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	1.95	0.47
1:A:429:GLN:N	1:A:886:GLN:HE22	2.10	0.47
1:A:1864:GLU:OE1	1:A:1890:LYS:NZ	2.37	0.47
1:B:442:TYR:HA	1:B:693:THR:HG23	1.95	0.47
1:B:971:LYS:HB2	1:B:980:GLN:HB2	1.96	0.47
1:B:1999:LEU:HD23	1:B:2000:THR:H	1.80	0.47
1:A:470:TYR:O	1:A:562:TYR:OH	2.23	0.47
1:A:1398:GLN:O	1:A:1402:ASN:HA	2.14	0.47
1:A:2015:PRO:HG2	1:A:2116:CYS:SG	2.54	0.47
1:B:1112:LEU:HG	1:B:1116:LYS:HE3	1.96	0.47
1:B:1225:VAL:O	1:B:1234:LEU:N	2.45	0.47
1:B:1405:VAL:HG22	1:B:1424:ILE:HB	1.96	0.47
1:A:760:GLU:HB2	1:A:805:HIS:ND1	2.29	0.47
1:A:600:GLY:HA2	1:A:907:LEU:HD23	1.95	0.47
1:A:741:MET:O	1:A:744:GLU:HG2	2.14	0.47
1:A:1923:ILE:HG21	1:A:1946:ALA:HB2	1.97	0.47
1:B:439:ARG:HD2	1:B:442:TYR:CZ	2.49	0.47
1:B:988:ALA:HA	1:B:993:ILE:HG12	1.97	0.47
1:B:2019:LEU:HD13	1:B:2041:LEU:HD23	1.96	0.47
1:B:1501:ALA:HB1	1:B:1506:CYS:HB2	1.96	0.47
1:A:423:MET:HE2	1:A:425:ASN:HB3	1.95	0.47
1:A:772:LEU:HG	1:A:773:GLU:HG3	1.96	0.47
1:A:1032:GLU:CD	1:A:1032:GLU:H	2.23	0.47
1:A:1339:VAL:HA	1:A:1486:ARG:HH22	1.80	0.47
1:A:1482:GLU:CD	1:A:1482:GLU:H	2.23	0.47
1:A:1870:GLN:O	1:A:1874:LYS:HG3	2.15	0.47
1:A:1595:LYS:HD3	1:B:666:ARG:NH1	2.28	0.47
1:A:1869:ARG:O	1:A:1873:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1993:ARG:O	1:A:1997:LEU:HB2	2.14	0.47
1:B:442:TYR:CD1	1:B:690:VAL:HG13	2.50	0.47
1:A:1660:LEU:HA	1:A:1701:ARG:O	2.15	0.46
1:B:858:ARG:HA	1:B:859:PRO:HD3	1.72	0.46
1:B:511:ASN:OD1	1:B:558:ARG:NH1	2.47	0.46
1:B:681:ARG:HH22	1:B:856:ALA:HB3	1.81	0.46
1:B:1366:ARG:O	1:B:1370:GLN:HG2	2.15	0.46
1:A:597:THR:HA	1:A:602:GLU:HB2	1.97	0.46
1:B:838:LYS:HA	1:B:838:LYS:HD3	1.65	0.46
1:B:901:LEU:O	1:B:905:ILE:HG12	2.15	0.46
1:B:1982:VAL:HG12	1:B:1983:PHE:H	1.81	0.46
1:A:540:TYR:OH	1:A:615:ASP:OD2	2.26	0.46
1:B:1346:VAL:HG13	1:B:1488:VAL:HG13	1.98	0.46
1:A:484:ILE:HG23	1:A:676:PHE:CE1	2.50	0.46
1:A:1477:ILE:O	1:A:1481:ILE:HG12	2.16	0.46
1:A:1595:LYS:HZ2	1:B:666:ARG:HE	1.61	0.46
1:B:1577:LEU:HD11	1:B:1615:ASN:HB2	1.97	0.46
1:B:2001:ASP:OD2	1:B:2002:SER:N	2.49	0.46
1:A:882:LEU:HD13	1:A:887:LEU:HD23	1.97	0.46
1:A:1052:ILE:HG13	1:A:1053:GLU:H	1.80	0.46
1:B:469:LYS:O	1:B:472:GLN:HG3	2.15	0.46
1:B:1180:LEU:O	1:B:1215:HIS:NE2	2.47	0.46
1:B:1301:LEU:HD22	1:B:1518:VAL:HB	1.97	0.46
1:B:1320:LEU:HD13	1:B:1396:LYS:HG2	1.97	0.46
1:A:838:LYS:O	1:A:840:ARG:HG3	2.16	0.46
1:B:1114:LEU:HA	1:B:1117:MET:HE3	1.98	0.46
1:B:1408:LEU:HD12	1:B:1427:SER:HB2	1.97	0.46
1:B:1729:ASP:HA	1:B:1732:MET:HE2	1.98	0.46
1:A:1501:ALA:HB1	1:A:1506:CYS:HB2	1.98	0.45
1:A:1970:HIS:CG	1:A:1971:ILE:N	2.84	0.45
1:B:422:PHE:CZ	1:B:935:LEU:HD11	2.52	0.45
1:B:853:LEU:HD12	1:B:883:LEU:HD22	1.98	0.45
1:B:1628:GLU:O	1:B:1632:VAL:HG23	2.17	0.45
1:A:1559:VAL:HG22	1:A:1660:LEU:HB3	1.97	0.45
1:B:482:ASN:O	1:B:486:SER:N	2.45	0.45
1:B:1131:GLN:HA	1:B:1133:ARG:HH12	1.81	0.45
1:A:1324:LYS:HG2	1:A:1325:PHE:HD1	1.80	0.45
1:B:772:LEU:HD21	1:B:786:HIS:HE2	1.81	0.45
1:B:1993:ARG:O	1:B:1999:LEU:HD13	2.16	0.45
1:A:432:ASP:HB3	1:A:433:GLY:H	1.55	0.45
1:A:2030:ARG:HG2	1:A:2031:SER:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:HA	1:A:431:PRO:HD3	1.85	0.45
1:A:1044:VAL:HA	1:A:1045:PRO:HD3	1.69	0.45
1:A:1201:GLU:HB3	1:A:1251:LEU:HD11	1.98	0.45
1:A:1581:ALA:HB2	1:A:1586:ARG:HD3	1.98	0.45
1:A:1980:GLU:N	1:A:1985:ILE:HD11	2.31	0.45
1:B:487:LYS:HD3	1:B:676:PHE:HE2	1.81	0.45
1:A:439:ARG:HD2	1:A:442:TYR:CZ	2.51	0.45
1:A:442:TYR:HA	1:A:693:THR:HG23	1.99	0.45
1:A:543:PRO:HB3	1:A:619:LEU:HD22	1.97	0.45
1:A:660:ASP:OD1	1:A:928:ARG:NH1	2.50	0.45
1:A:1049:LYS:HD3	1:A:1049:LYS:HA	1.83	0.45
1:A:2064:TRP:NE1	1:A:2084:LEU:HD23	2.32	0.45
1:B:1514:PHE:HB3	1:B:1518:VAL:CG2	2.46	0.45
1:A:681:ARG:HG3	1:A:682:PRO:HD2	1.99	0.45
1:A:687:GLN:OE1	1:A:689:TYR:OH	2.12	0.45
1:A:1158:HIS:CG	1:A:1172:LYS:HG2	2.52	0.45
1:A:2019:LEU:HD11	1:A:2039:VAL:HG12	1.99	0.45
1:A:844:LEU:HB3	1:A:849:ILE:HD11	1.99	0.45
1:B:1154:TYR:CE1	1:B:1183:LYS:HD2	2.52	0.45
1:B:1201:GLU:HB3	1:B:1251:LEU:HD11	1.98	0.45
1:B:1312:LEU:HD21	1:B:1317:PHE:HB3	1.98	0.45
1:A:641:MET:HG2	1:A:1582:ALA:CB	2.47	0.44
1:A:1053:GLU:OE1	1:A:1053:GLU:N	2.50	0.44
1:A:2080:LYS:HB2	1:A:2080:LYS:HE3	1.68	0.44
1:B:1320:LEU:HA	1:B:1400:ARG:NH2	2.32	0.44
1:A:1568:GLN:OE1	1:A:1664:MET:HE1	2.18	0.44
1:B:1314:ASN:O	1:B:1318:GLU:HG3	2.17	0.44
1:B:1861:ARG:NH1	1:B:1907:GLU:HB3	2.32	0.44
1:A:1066:PHE:CG	1:A:1085:THR:HG21	2.53	0.44
1:A:1515:HIS:O	1:A:1518:VAL:HG22	2.17	0.44
1:A:1351:PRO:CG	1:A:1516:PRO:HA	2.45	0.44
1:A:2018:GLU:H	1:A:2043:ARG:CZ	2.30	0.44
1:B:484:ILE:HG23	1:B:676:PHE:CE1	2.53	0.44
1:B:1142:LYS:HG2	1:B:1167:MET:HE3	2.00	0.44
1:B:1411:GLU:OE1	1:B:1414:THR:OG1	2.30	0.44
1:B:1496:ASN:OD1	1:B:1496:ASN:N	2.50	0.44
1:B:2023:VAL:HG22	1:B:2037:VAL:HG22	1.99	0.44
1:A:924:TYR:CZ	1:A:928:ARG:HD3	2.52	0.44
1:B:1433:ASP:OD1	1:B:1823:TYR:OH	2.24	0.44
1:A:482:ASN:H	1:A:485:GLN:NE2	2.15	0.44
1:A:681:ARG:NH1	1:A:685:LEU:HD22	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:HIS:HB2	1:A:1172:LYS:HA	2.00	0.44
1:A:1455:GLU:O	1:A:1458:LEU:HB2	2.17	0.44
1:A:2016:ASN:O	1:A:2043:ARG:HD2	2.18	0.44
1:A:2051:VAL:HG22	1:A:2062:GLU:HG2	2.00	0.44
1:B:434:SER:N	3:B:2606:HOH:O	2.51	0.44
1:B:1378:TYR:OH	1:B:1454:ASP:OD2	2.34	0.44
1:A:1433:ASP:OD2	1:A:1473:ARG:NH2	2.51	0.44
1:A:1973:ARG:HG3	1:A:1974:CYS:H	1.82	0.44
1:B:844:LEU:HD23	1:B:849:ILE:HG12	1.98	0.44
1:A:1314:ASN:HB3	1:A:1317:PHE:CD2	2.53	0.43
1:B:443:GLU:OE1	1:B:873:HIS:NE2	2.47	0.43
1:B:1439:TRP:CD1	1:B:1473:ARG:HD2	2.53	0.43
1:B:1498:LYS:HE3	1:B:1498:LYS:HB2	1.73	0.43
1:B:1553:HIS:O	1:B:1701:ARG:NH1	2.50	0.43
1:B:1559:VAL:HG22	1:B:1660:LEU:HB3	2.00	0.43
1:B:1761:TYR:CE2	1:B:1781:LEU:HD21	2.53	0.43
1:A:1745:ILE:HA	1:A:1750:ASP:HB3	2.00	0.43
1:B:1307:LEU:HB3	1:B:1333:THR:HG22	1.99	0.43
1:B:1375:ARG:HD3	1:B:1422:GLY:O	2.18	0.43
1:B:1397:PHE:HB2	1:B:1405:VAL:HG21	2.01	0.43
1:A:752:LEU:HD13	1:A:782:PHE:HE2	1.83	0.43
1:A:1269:ARG:NH1	1:A:1279:GLU:OE2	2.51	0.43
1:B:464:VAL:O	1:B:467:LEU:HG	2.18	0.43
1:B:526:ASN:O	1:B:528:ASP:N	2.51	0.43
1:B:547:LEU:HD11	1:B:551:MET:HE2	2.01	0.43
1:B:1930:LEU:HD22	1:B:1938:PRO:HB2	2.01	0.43
1:A:1861:ARG:CZ	1:A:1907:GLU:HB3	2.48	0.43
1:B:917:VAL:HG13	1:B:953:ARG:HB3	2.00	0.43
1:B:2019:LEU:HD11	1:B:2039:VAL:HG12	1.99	0.43
1:A:1943:MET:HE1	1:A:2067:VAL:HG21	2.01	0.43
1:A:2019:LEU:HD12	1:A:2019:LEU:HA	1.79	0.43
1:B:591:GLU:HG3	2:B:2501:8LV:C10	2.47	0.43
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.59	0.43
1:A:533:VAL:HG13	1:A:584:GLN:NE2	2.34	0.43
1:A:734:THR:O	1:A:738:ILE:HG12	2.19	0.43
1:A:1865:ASP:OD1	1:A:1865:ASP:N	2.52	0.43
1:A:1970:HIS:ND1	1:A:1971:ILE:HG12	2.34	0.43
1:A:2043:ARG:HG3	1:A:2044:GLU:O	2.19	0.43
1:B:1796:LEU:HB3	1:B:1802:ILE:HG12	2.00	0.43
1:A:933:PRO:HG3	1:A:943:LEU:HD22	2.00	0.43
1:A:1329:ASN:O	1:A:1333:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1473:ARG:NH1	1:A:1739:GLU:OE2	2.52	0.43
1:A:1618:GLY:O	1:A:1644:VAL:HA	2.18	0.43
1:A:2039:VAL:HB	1:A:2090:VAL:HB	2.01	0.43
1:B:1084:VAL:HG23	1:B:1085:THR:HG23	2.00	0.43
1:B:1404:LYS:HA	1:B:1404:LYS:HD3	1.88	0.43
1:A:750:LEU:HD12	1:A:750:LEU:HA	1.92	0.43
1:A:1093:ARG:NH2	1:A:1115:CYS:HB3	2.33	0.43
1:A:1456:VAL:CG2	1:A:1491:SER:HB2	2.43	0.43
1:B:681:ARG:NH1	1:B:685:LEU:HD22	2.34	0.43
1:A:1018:PHE:CE2	1:A:1063:LEU:HD22	2.55	0.42
1:B:533:VAL:HG13	1:B:584:GLN:NE2	2.34	0.42
1:B:1666:THR:HG21	1:B:1714:PHE:CE1	2.54	0.42
1:B:2059:LYS:HA	1:B:2059:LYS:HD2	1.91	0.42
1:A:1007:PRO:HG3	1:A:1104:TRP:CE2	2.54	0.42
1:A:1566:ARG:HG3	1:A:1621:HIS:CG	2.54	0.42
1:B:642:THR:C	1:B:644:GLU:H	2.27	0.42
1:B:1382:MET:HE3	1:B:1652:TRP:CE2	2.54	0.42
1:A:784:ILE:HA	1:A:810:VAL:O	2.18	0.42
1:B:1542:MET:C	1:B:1545:PRO:HD2	2.44	0.42
1:B:1859:PRO:O	1:B:1890:LYS:NZ	2.47	0.42
1:A:922:TYR:CD2	1:B:1595:LYS:HE2	2.55	0.42
1:A:1204:ILE:HD12	1:A:1252:ILE:HD13	2.01	0.42
1:A:1260:GLU:O	1:A:1262:LEU:N	2.52	0.42
1:B:1558:PRO:HB3	3:B:2629:HOH:O	2.19	0.42
1:A:742:CYS:O	1:A:749:GLY:N	2.52	0.42
1:A:1225:VAL:O	1:A:1234:LEU:N	2.48	0.42
1:B:676:PHE:HB3	1:B:680:PHE:CG	2.55	0.42
1:A:545:ARG:H	2:A:2501:8LV:C19	2.33	0.42
1:A:759:THR:HB	1:A:760:GLU:H	1.41	0.42
1:A:1432:TRP:HE1	1:A:1474:MET:HE3	1.84	0.42
1:A:1586:ARG:C	1:A:1588:ARG:H	2.28	0.42
1:A:2017:ILE:HD13	1:A:2108:PHE:CE2	2.54	0.42
1:B:632:VAL:O	1:B:636:ILE:HG12	2.19	0.42
1:B:1777:SER:OG	1:B:1780:HIS:ND1	2.46	0.42
1:B:1843:ARG:HD3	1:B:1877:HIS:CG	2.54	0.42
1:B:1937:SER:OG	1:B:1938:PRO:HD3	2.19	0.42
1:A:1093:ARG:HH21	1:A:1115:CYS:HB3	1.85	0.42
1:A:1560:ILE:HG13	1:A:1658:ALA:HB2	2.02	0.42
1:B:772:LEU:HD22	1:B:789:MET:HG2	2.00	0.42
1:B:882:LEU:HD13	1:B:887:LEU:HD23	2.02	0.42
1:B:1735:HIS:O	1:B:1739:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:THR:HG21	1:A:676:PHE:O	2.20	0.42
1:A:1142:LYS:HG2	1:A:1167:MET:HE3	2.02	0.42
1:A:1598:ILE:HB	1:A:1599:PRO:HD3	2.00	0.42
1:A:2051:VAL:HG13	1:A:2113:TYR:CZ	2.54	0.42
1:B:439:ARG:HD2	1:B:442:TYR:OH	2.19	0.42
1:A:712:ILE:HD13	1:A:721:VAL:HG11	2.02	0.42
1:B:516:CYS:SG	1:B:649:ILE:HG12	2.60	0.42
1:B:1829:ILE:H	1:B:1829:ILE:HG13	1.68	0.42
1:A:1274:ARG:HD2	1:A:1274:ARG:HA	1.84	0.42
1:A:1962:GLN:HE22	1:A:2114:MET:H	1.67	0.42
1:B:611:LEU:HD11	1:B:649:ILE:HD13	2.02	0.42
1:A:690:VAL:HG21	1:A:707:ILE:HG21	2.01	0.41
1:A:744:GLU:HB3	1:A:745:LYS:H	1.35	0.41
1:A:1062:LEU:HD23	1:A:1062:LEU:HA	1.86	0.41
1:A:1136:PRO:HB2	1:A:1139:VAL:HG23	2.01	0.41
1:A:1725:GLU:HB3	1:A:1771:TYR:OH	2.19	0.41
1:B:728:ARG:HG3	1:B:1075:PHE:HE1	1.85	0.41
1:B:1149:PRO:HG2	1:B:1152:ARG:HG3	2.02	0.41
1:B:1796:LEU:HD23	1:B:1796:LEU:HA	1.94	0.41
1:B:2064:TRP:CZ3	1:B:2110:SER:HB2	2.55	0.41
1:A:632:VAL:O	1:A:636:ILE:HG12	2.20	0.41
1:A:666:ARG:HE	1:B:1595:LYS:HZ3	1.65	0.41
1:A:991:TYR:CE1	1:A:1097:GLU:HG3	2.55	0.41
1:A:1112:LEU:O	1:A:1116:LYS:HG3	2.19	0.41
1:A:1755:LEU:HD23	1:A:1755:LEU:HA	1.88	0.41
1:B:899:ASP:OD1	1:B:995:ASN:ND2	2.46	0.41
1:B:1223:ILE:HG12	1:B:1270:VAL:HG22	2.01	0.41
1:B:1225:VAL:HG11	1:B:1256:VAL:HG11	2.01	0.41
1:B:1314:ASN:HB3	1:B:1317:PHE:CD2	2.55	0.41
1:B:1985:ILE:HA	1:B:1988:MET:HE3	2.02	0.41
1:A:422:PHE:HZ	1:A:935:LEU:HD11	1.86	0.41
1:A:887:LEU:HA	1:A:888:PRO:HD3	1.87	0.41
1:A:1153:LEU:HD23	1:A:1153:LEU:HA	1.89	0.41
1:B:1157:ASN:ND2	1:B:1159:ASN:HB2	2.36	0.41
1:B:1347:PHE:HZ	1:B:1494:LEU:HD12	1.85	0.41
1:B:1361:GLU:O	1:B:1365:LEU:HG	2.21	0.41
1:A:469:LYS:O	1:A:472:GLN:HG3	2.20	0.41
1:A:1519:ARG:NH1	1:A:1523:LEU:HB2	2.36	0.41
1:B:1843:ARG:HH11	1:B:1877:HIS:CE1	2.39	0.41
1:A:642:THR:C	1:A:644:GLU:H	2.28	0.41
1:A:1276:LEU:HD23	1:A:1276:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1338:THR:O	1:A:1342:SER:HB2	2.20	0.41
1:A:1514:PHE:HB3	1:A:1518:VAL:CG2	2.50	0.41
1:B:639:ILE:HD11	1:B:646:VAL:HB	2.03	0.41
1:B:1112:LEU:O	1:B:1116:LYS:HG3	2.21	0.41
1:B:1299:THR:N	1:B:1513:ASN:O	2.53	0.41
1:B:1907:GLU:OE1	1:B:1907:GLU:N	2.51	0.41
1:B:2070:ASP:OD1	1:B:2072:LYS:HE2	2.20	0.41
1:B:1432:TRP:HE1	1:B:1474:MET:HE3	1.85	0.41
1:B:1945:LEU:HA	1:B:1948:MET:HG2	2.01	0.41
1:B:2046:GLU:HG3	1:B:2086:GLN:OE1	2.20	0.41
1:A:517:MET:HE2	1:A:559:LEU:HD11	2.02	0.41
1:A:853:LEU:HA	1:A:853:LEU:HD23	1.74	0.41
1:A:1614:LEU:HA	1:A:1614:LEU:HD23	1.74	0.41
1:B:578:GLU:HA	1:B:581:SER:OG	2.20	0.41
1:B:1062:LEU:HA	1:B:1062:LEU:HD23	1.84	0.41
1:B:1473:ARG:NH1	1:B:1739:GLU:OE2	2.54	0.41
1:B:1755:LEU:HD13	1:B:1785:LEU:HD22	2.03	0.41
1:B:499:LEU:HB2	1:B:649:ILE:HG13	2.03	0.41
1:B:1432:TRP:HE1	1:B:1474:MET:CE	2.33	0.41
1:B:1481:ILE:HG13	1:B:1482:GLU:N	2.36	0.41
1:B:1566:ARG:HG3	1:B:1621:HIS:CG	2.56	0.41
1:B:1614:LEU:HD23	1:B:1614:LEU:HA	1.84	0.41
1:B:1747:ASN:O	1:B:1750:ASP:HB2	2.21	0.41
1:B:1876:PRO:HG2	1:B:1954:TRP:CE2	2.56	0.41
1:A:439:ARG:C	1:A:441:GLY:H	2.29	0.41
1:A:509:LYS:H	1:A:509:LYS:HG2	1.68	0.41
1:A:533:VAL:HG13	1:A:584:GLN:CD	2.46	0.41
1:A:591:GLU:HG3	2:A:2501:8LV:C10	2.50	0.41
1:A:763:ARG:O	1:A:767:GLU:HG2	2.19	0.41
1:A:850:LEU:HD23	1:A:883:LEU:HD23	2.03	0.41
1:A:1183:LYS:HB3	1:A:1207:ASP:O	2.21	0.41
1:A:1301:LEU:HD22	1:A:1518:VAL:HB	2.03	0.41
1:A:1766:GLN:HE21	1:A:1766:GLN:HA	1.86	0.41
1:B:834:TYR:OH	1:B:1080:ASP:OD1	2.36	0.41
1:B:1336:PHE:HD2	1:B:1362:PHE:CE2	2.39	0.41
1:B:1542:MET:O	1:B:1546:VAL:HG23	2.21	0.41
1:B:1714:PHE:O	1:B:1718:LEU:HB2	2.20	0.41
1:B:1822:TYR:O	1:B:1921:ARG:HD3	2.21	0.41
1:A:569:LEU:HD12	1:A:569:LEU:HA	1.93	0.41
1:A:607:GLN:HG3	1:A:608:LEU:HD13	2.03	0.41
1:A:1331:ILE:HD12	1:A:1514:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2068:ILE:HG22	1:A:2077:ILE:HB	2.02	0.41
1:B:1627:MET:HE3	1:B:1627:MET:HB3	1.95	0.41
1:B:1865:ASP:N	1:B:1865:ASP:OD1	2.54	0.41
1:A:425:ASN:HB2	1:A:888:PRO:HD3	2.03	0.40
1:A:517:MET:HG2	1:A:538:ILE:HG21	2.03	0.40
1:A:617:ILE:CG2	1:A:652:SER:HB2	2.51	0.40
1:A:948:LEU:O	1:A:953:ARG:NH1	2.53	0.40
1:A:1013:GLU:O	1:A:1017:VAL:HG23	2.20	0.40
1:A:1628:GLU:O	1:A:1632:VAL:HG23	2.21	0.40
1:B:548:VAL:HG13	1:B:587:VAL:HG12	2.03	0.40
1:B:838:LYS:O	1:B:840:ARG:HG3	2.21	0.40
1:A:487:LYS:HD3	1:A:676:PHE:CE2	2.56	0.40
1:B:618:HIS:C	1:B:620:LEU:N	2.79	0.40
1:B:2021:TYR:OH	1:B:2122:PHE:HB3	2.21	0.40
1:A:1223:ILE:HG12	1:A:1270:VAL:HG22	2.01	0.40
1:A:1829:ILE:H	1:A:1829:ILE:HG13	1.68	0.40
1:B:869:LEU:HD23	1:B:879:TYR:HB3	2.03	0.40
1:B:1407:LEU:HD12	1:B:1426:ILE:HB	2.04	0.40
1:B:1769:ASN:HD22	1:B:1769:ASN:HA	1.66	0.40
1:A:962:LEU:HD23	1:A:962:LEU:HA	1.90	0.40
1:A:1303:ASP:OD2	1:A:1303:ASP:N	2.54	0.40
1:B:483:ARG:HE	1:B:680:PHE:HE1	1.69	0.40
1:B:1046:ILE:HB	1:B:1064:GLN:NE2	2.37	0.40
1:B:1901:ARG:HD2	1:B:1961:LYS:HE2	2.04	0.40
1:A:1886:ASP:HA	1:A:1887:PRO:HD2	1.95	0.40
1:B:753:ARG:HD2	1:B:761:VAL:HG13	2.02	0.40
1:B:1455:GLU:O	1:B:1458:LEU:HB2	2.21	0.40
1:B:2035:VAL:CG2	1:B:2096:ALA:HB2	2.52	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	1714/1738 (99%)	1633 (95%)	75 (4%)	6 (0%)	30	60
1	B	1677/1738 (96%)	1603 (96%)	70 (4%)	4 (0%)	43	72
All	All	3391/3476 (98%)	3236 (95%)	145 (4%)	10 (0%)	36	66

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1989	GLU
1	B	1050	GLU
1	A	1050	GLU
1	A	1665	ASP
1	B	1665	ASP
1	A	2026	LYS
1	A	1052	ILE
1	B	1052	ILE
1	A	1584	ILE
1	B	1584	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1534/1551 (99%)	1501 (98%)	33 (2%)	45	78
1	B	1514/1551 (98%)	1484 (98%)	30 (2%)	48	80
All	All	3048/3102 (98%)	2985 (98%)	63 (2%)	47	79

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	462	LEU
1	A	489	TYR
1	A	510	THR
1	A	533	VAL
1	A	545	ARG
1	A	546	SER

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Mol	Chain	Res	Type
1	A	585	ILE
1	A	591	GLU
1	A	602	GLU
1	A	610	ARG
1	A	667	VAL
1	A	759	THR
1	A	760	GLU
1	A	773	GLU
1	A	849	ILE
1	A	871	THR
1	A	875	GLU
1	A	876	LEU
1	A	998	VAL
1	A	1307	LEU
1	A	1577	LEU
1	A	1656	VAL
1	A	1696	GLN
1	A	1829	ILE
1	A	1842	VAL
1	A	1862	HIS
1	A	1973	ARG
1	A	1982	VAL
1	A	2000	THR
1	A	2023	VAL
1	A	2080	LYS
1	A	2084	LEU
1	A	2090	VAL
1	B	462	LEU
1	B	531	ILE
1	B	533	VAL
1	B	546	SER
1	B	585	ILE
1	B	591	GLU
1	B	602	GLU
1	B	610	ARG
1	B	770	LYS
1	B	773	GLU
1	B	778	LEU
1	B	792	VAL
1	B	809	LEU
1	B	876	LEU
1	B	939	SER

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Mol	Chain	Res	Type
1	B	998	VAL
1	B	1170	MET
1	B	1252	ILE
1	B	1265	GLN
1	B	1380	THR
1	B	1453	VAL
1	B	1575	ASP
1	B	1577	LEU
1	B	1656	VAL
1	B	1696	GLN
1	B	1829	ILE
1	B	1842	VAL
1	B	1862	HIS
1	B	1982	VAL
1	B	2084	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	GLN
1	A	526	ASN
1	A	532	ASN
1	A	832	GLN
1	A	877	GLN
1	A	951	GLN
1	A	978	ASN
1	A	999	GLN
1	A	1003	GLN
1	A	1101	ASN
1	A	1236	HIS
1	A	1553	HIS
1	A	1667	GLN
1	A	1674	HIS
1	A	1690	HIS
1	A	1692	ASN
1	A	1877	HIS
1	A	2040	GLN
1	A	2118	GLN
1	B	425	ASN
1	B	532	ASN
1	B	715	HIS
1	B	951	GLN

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Mol	Chain	Res	Type
1	B	1003	GLN
1	B	1322	GLN
1	B	1568	GLN
1	B	1667	GLN
1	B	1692	ASN
1	B	1778	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	8LV	A	2501	-	31,36,36	1.12	1 (3%)	32,52,52	1.77	7 (21%)
2	8LV	B	2501	-	31,36,36	1.17	1 (3%)	32,52,52	1.58	6 (18%)

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	8LV	A	2501	-	-	6/12/32/32	0/5/5/5
2	8LV	B	2501	-	-	4/12/32/32	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2501	8LV	C16-C15	4.16	1.49	1.45
2	A	2501	8LV	C16-C15	4.05	1.49	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2501	8LV	C14-C13-C12	-4.38	126.01	133.96
2	A	2501	8LV	O32-C13-C14	3.93	124.09	116.61
2	B	2501	8LV	C14-C13-C12	-3.72	127.22	133.96
2	A	2501	8LV	O32-C10-C8	3.49	120.86	116.73
2	A	2501	8LV	C14-C15-C16	3.43	122.97	117.23
2	B	2501	8LV	O32-C13-C14	2.82	121.98	116.61
2	B	2501	8LV	C14-C15-C16	2.81	121.93	117.23
2	B	2501	8LV	C7-C8-C10	-2.65	116.55	120.77
2	B	2501	8LV	O32-C10-C8	2.62	119.83	116.73
2	A	2501	8LV	C7-C8-C10	-2.23	117.23	120.77
2	B	2501	8LV	C10-O32-C13	-2.09	105.81	106.93
2	A	2501	8LV	C9-C8-C10	2.06	123.58	120.25
2	A	2501	8LV	O1-C2-O3	2.02	127.69	123.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

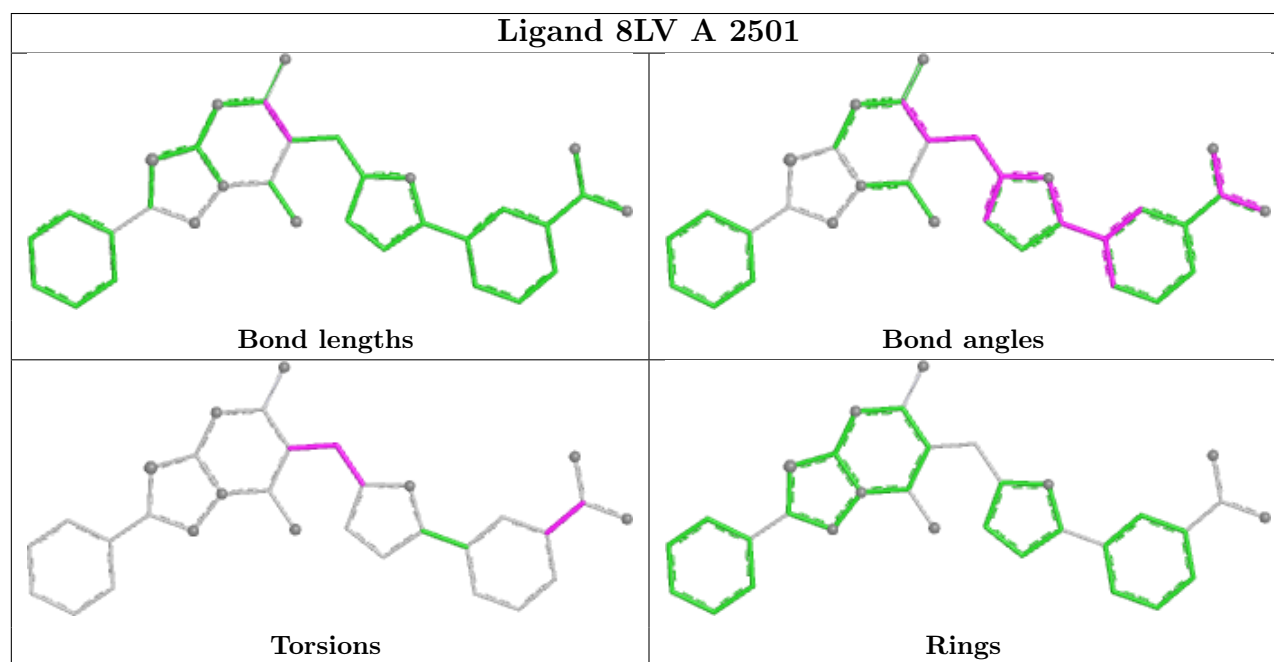
Mol	Chain	Res	Type	Atoms
2	A	2501	8LV	C13-C14-C15-C24
2	A	2501	8LV	C13-C14-C15-C16
2	B	2501	8LV	C13-C14-C15-C24
2	B	2501	8LV	C13-C14-C15-C16
2	A	2501	8LV	C12-C13-C14-C15
2	B	2501	8LV	C12-C13-C14-C15
2	A	2501	8LV	O32-C13-C14-C15
2	B	2501	8LV	O32-C13-C14-C15
2	A	2501	8LV	O3-C2-C4-C9
2	A	2501	8LV	O3-C2-C4-C5

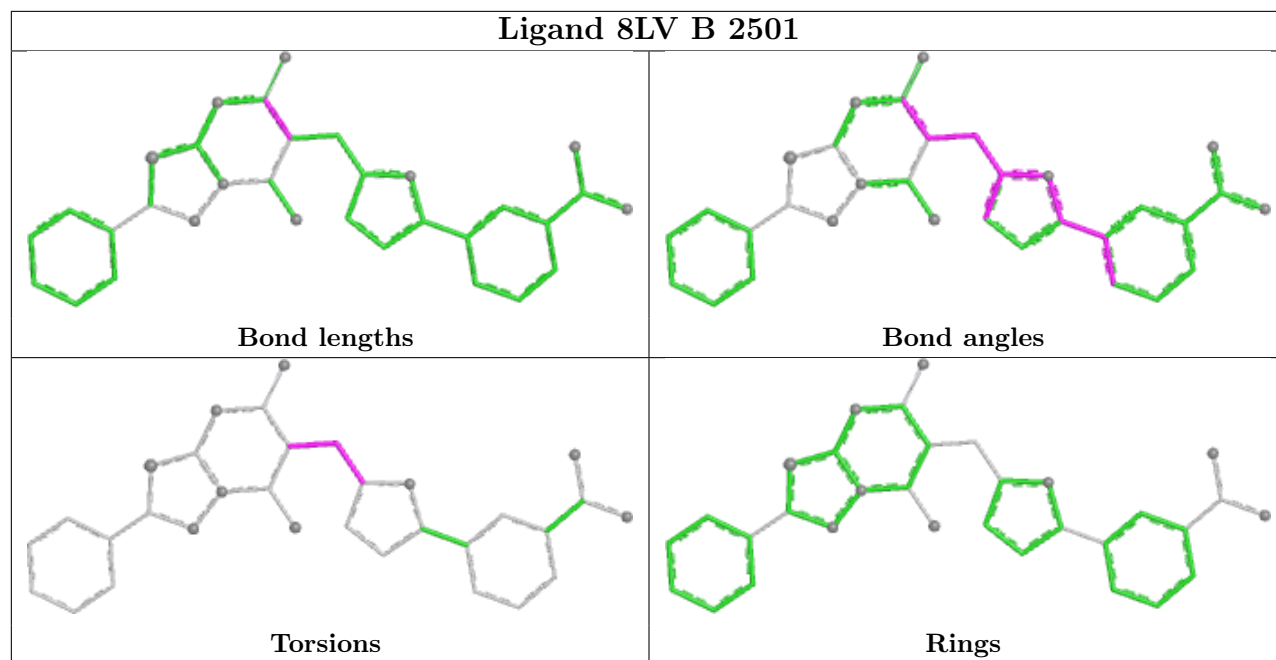
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2501	8LV	3	0
2	B	2501	8LV	2	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	1718/1738 (98%)	0.32	79 (4%) 37 29	41, 71, 126, 176	0
1	B	1691/1738 (97%)	0.43	83 (4%) 35 27	46, 76, 122, 160	0
All	All	3409/3476 (98%)	0.37	162 (4%) 35 28	41, 74, 123, 176	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	751	PHE	5.9
1	B	1982	VAL	5.7
1	A	771	ASN	4.0
1	A	758	SER	4.0
1	B	753	ARG	4.0
1	B	761	VAL	4.0
1	A	748	LEU	3.8
1	A	1999	LEU	3.8
1	A	1982	VAL	3.7
1	B	2112	ALA	3.6
1	A	1986	MET	3.5
1	B	844	LEU	3.5
1	A	1587	GLN	3.5
1	B	2042	GLU	3.4
1	B	441	GLY	3.4
1	B	574	GLN	3.4
1	B	1317	PHE	3.4
1	A	743	LEU	3.4
1	A	1050	GLU	3.4
1	A	1973	ARG	3.4
1	B	748	LEU	3.3
1	B	772	LEU	3.2
1	B	739	ARG	3.2
1	B	862	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	757	ALA	3.2
1	B	863	THR	3.2
1	A	1985	ILE	3.2
1	B	1050	GLU	3.2
1	A	1983	PHE	3.1
1	A	1342	SER	3.1
1	A	2004	ILE	3.1
1	A	755	GLY	3.1
1	B	754	GLU	3.1
1	A	1975	THR	3.1
1	A	2024	VAL	3.0
1	A	530	THR	3.0
1	A	2084	LEU	3.0
1	B	573	HIS	3.0
1	A	772	LEU	2.9
1	B	861	TYR	2.9
1	B	747	THR	2.9
1	B	461	LEU	2.9
1	A	751	PHE	2.9
1	A	1996	LEU	2.9
1	B	2017	ILE	2.9
1	A	2047	VAL	2.8
1	B	570	THR	2.8
1	B	1342	SER	2.8
1	B	1247	GLN	2.8
1	A	753	ARG	2.8
1	B	694	GLU	2.8
1	A	2098	ALA	2.7
1	B	693	THR	2.7
1	B	750	LEU	2.7
1	A	2043	ARG	2.7
1	B	1312	LEU	2.7
1	B	1999	LEU	2.7
1	B	455	PHE	2.7
1	A	1993	ARG	2.7
1	B	530	THR	2.7
1	A	2007	VAL	2.7
1	A	770	LYS	2.6
1	B	746	ASP	2.6
1	A	1051	SER	2.6
1	B	2005	ALA	2.6
1	B	2020	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1997	LEU	2.6
1	A	756	SER	2.6
1	B	764	THR	2.6
1	B	1587	GLN	2.6
1	A	574	GLN	2.5
1	B	745	LYS	2.5
1	A	752	LEU	2.5
1	B	531	ILE	2.5
1	B	715	HIS	2.5
1	B	1964	PRO	2.5
1	B	437	ARG	2.5
1	B	473	ALA	2.5
1	B	1316	ALA	2.5
1	A	2041	LEU	2.4
1	A	2124	VAL	2.4
1	A	432	ASP	2.4
1	B	2047	VAL	2.4
1	B	2043	ARG	2.4
1	B	1400	ARG	2.4
1	A	2088	ALA	2.4
1	B	787	ALA	2.4
1	B	1774	GLN	2.4
1	B	741	MET	2.4
1	A	464	VAL	2.4
1	B	1779	ARG	2.4
1	A	2052	ILE	2.4
1	A	941	ASP	2.3
1	B	1966	PHE	2.3
1	A	1953	MET	2.3
1	A	1288	HIS	2.3
1	A	761	VAL	2.3
1	A	645	ASP	2.3
1	B	2086	GLN	2.3
1	B	1985	ILE	2.3
1	B	2014	TYR	2.3
1	B	453	LYS	2.3
1	A	2042	GLU	2.3
1	B	713	MET	2.3
1	A	1960	LEU	2.3
1	A	2003	GLN	2.3
1	B	821	LEU	2.3
1	B	1051	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1994	ASN	2.2
1	A	2011	CYS	2.2
1	A	759	THR	2.2
1	A	2023	VAL	2.2
1	A	1995	ALA	2.2
1	A	2017	ILE	2.2
1	A	437	ARG	2.2
1	B	454	PRO	2.2
1	B	2124	VAL	2.2
1	B	2024	VAL	2.2
1	B	2100	GLY	2.2
1	A	493	LEU	2.2
1	B	1365	LEU	2.2
1	A	694	GLU	2.2
1	A	763	ARG	2.2
1	B	2003	GLN	2.2
1	A	1970	HIS	2.2
1	B	2021	TYR	2.2
1	A	462	LEU	2.2
1	A	1958	SER	2.2
1	B	691	GLY	2.1
1	B	1420	GLY	2.1
1	A	2038	LEU	2.1
1	A	1260	GLU	2.1
1	B	2036	VAL	2.1
1	B	804	LYS	2.1
1	B	433	GLY	2.1
1	A	2010	PHE	2.1
1	A	2112	ALA	2.1
1	A	1039	LYS	2.1
1	B	1327	PHE	2.1
1	A	412	GLU	2.1
1	A	578	GLU	2.1
1	A	2029	ILE	2.1
1	B	602	GLU	2.1
1	B	765	GLU	2.1
1	A	573	HIS	2.1
1	A	2114	MET	2.1
1	A	425	ASN	2.1
1	A	570	THR	2.1
1	A	740	ASP	2.1
1	A	1992	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	875	GLU	2.1
1	A	939	SER	2.0
1	B	2002	SER	2.0
1	B	2087	LYS	2.0
1	B	752	LEU	2.0
1	B	1963	LEU	2.0
1	A	1959	TYR	2.0
1	B	1322	GLN	2.0
1	B	463	PRO	2.0
1	B	1369	LEU	2.0
1	A	1966	PHE	2.0
1	B	571	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

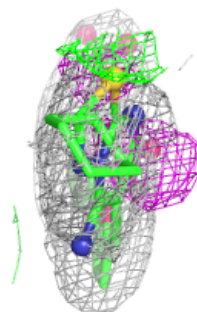
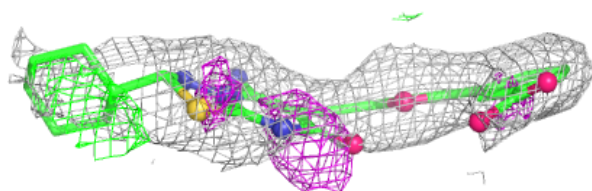
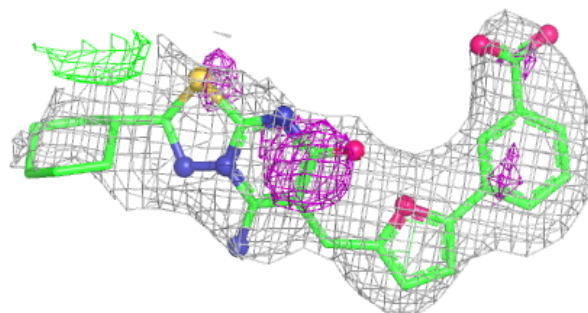
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	8LV	B	2501	32/32	0.74	0.16	64,88,112,117	0
2	8LV	A	2501	32/32	0.86	0.11	58,75,81,83	0

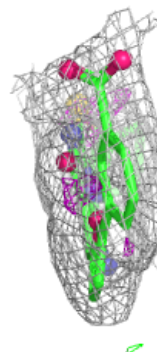
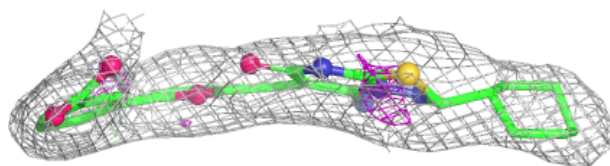
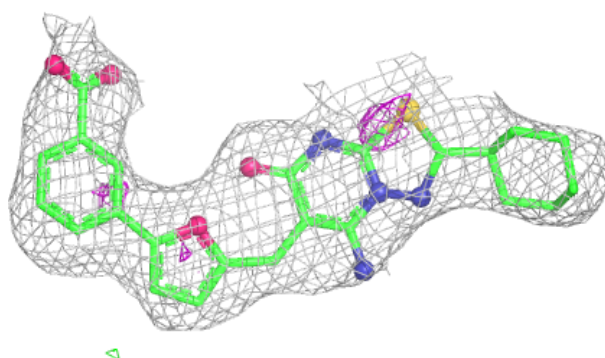
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8LV B 2501:

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

**Electron density around 8LV A 2501:**

$2mF_o-DF_c$ (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.