



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 07:44 PM EDT

PDB ID : 5URM
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

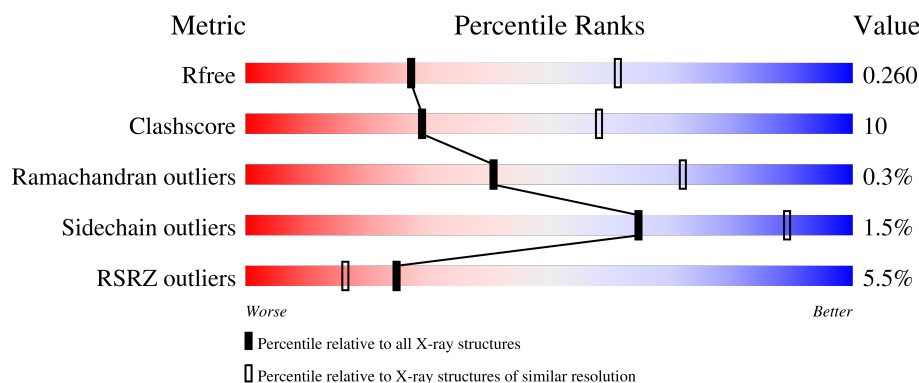
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>..</div> </div> </div>
1	B	1738	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>..</div> </div> </div>

2 Entry composition

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.

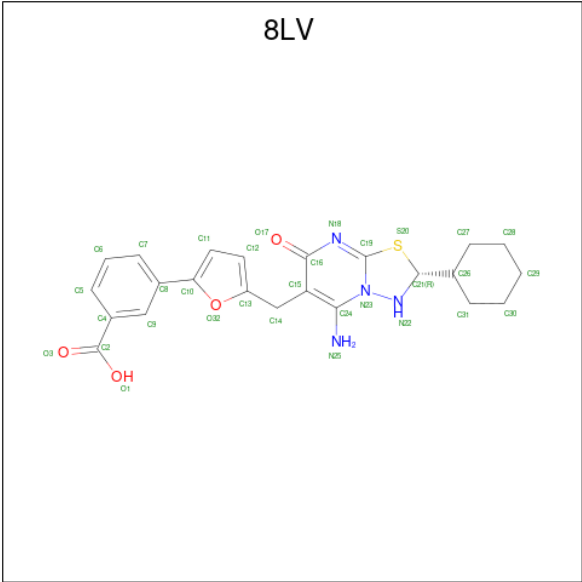
- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

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 (three-letter code: 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		

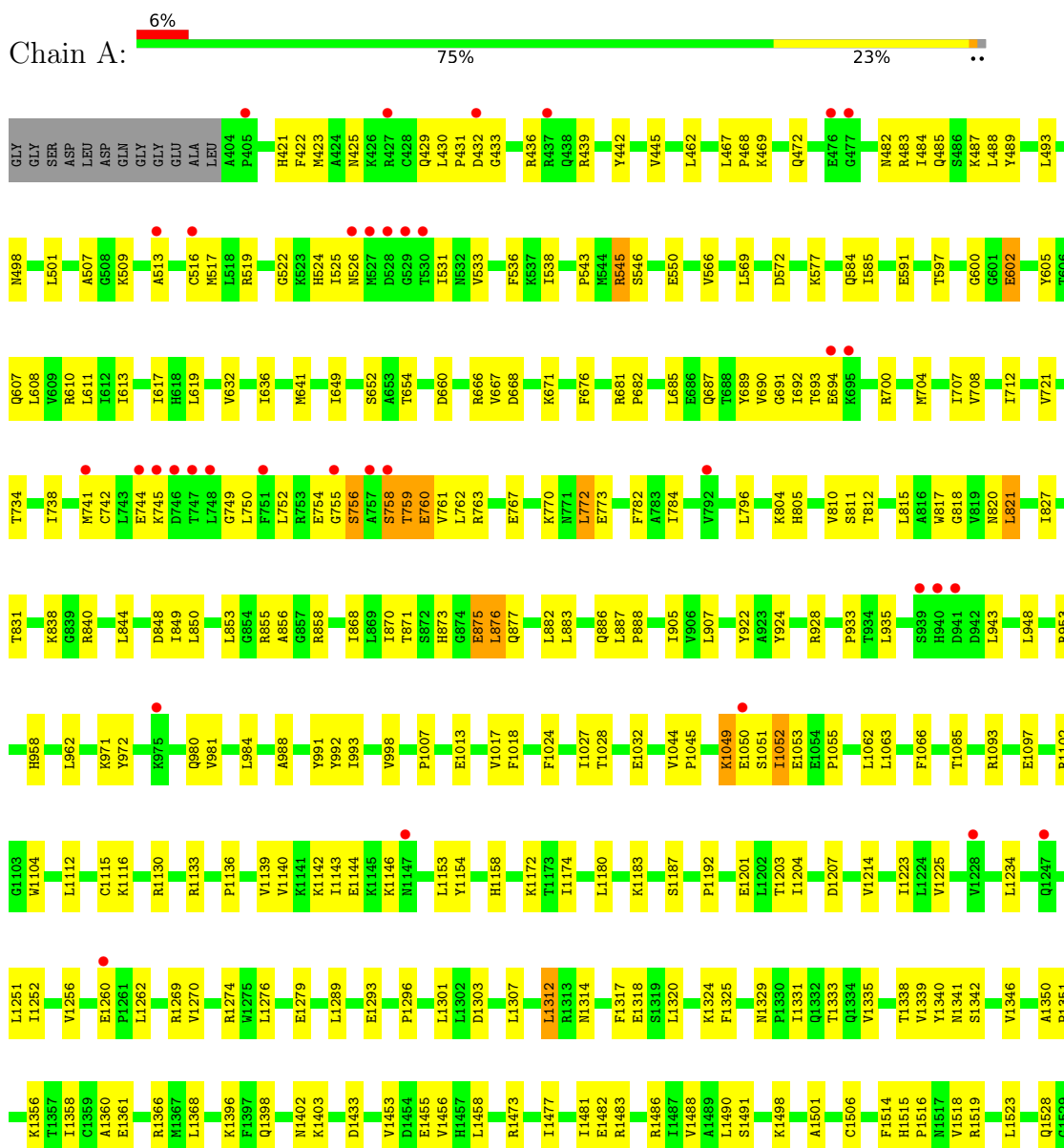
- Molecule 3 is water.

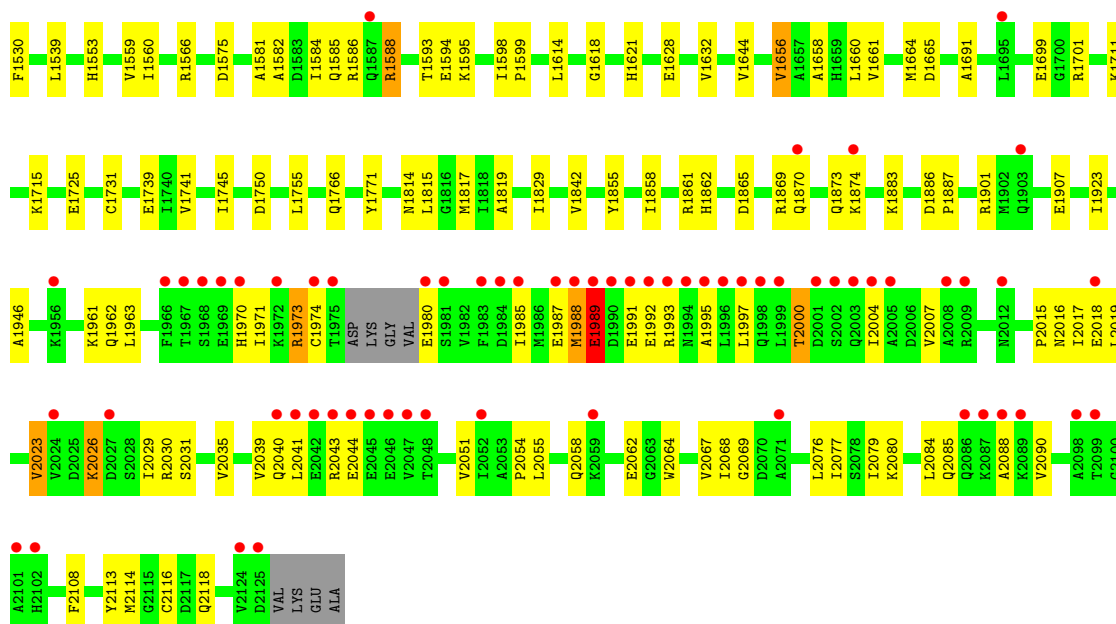
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	44	Total	O	0	0
			44	44		

3 Residue-property plots [i](#)

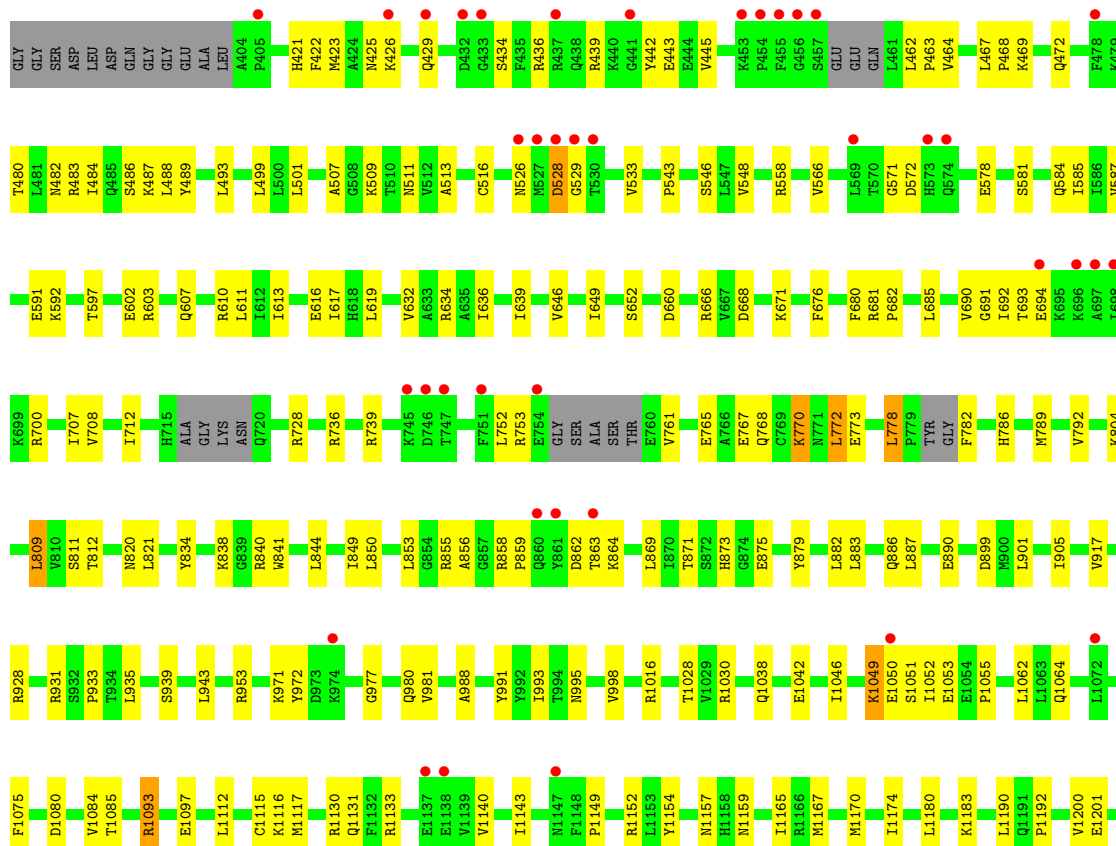
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

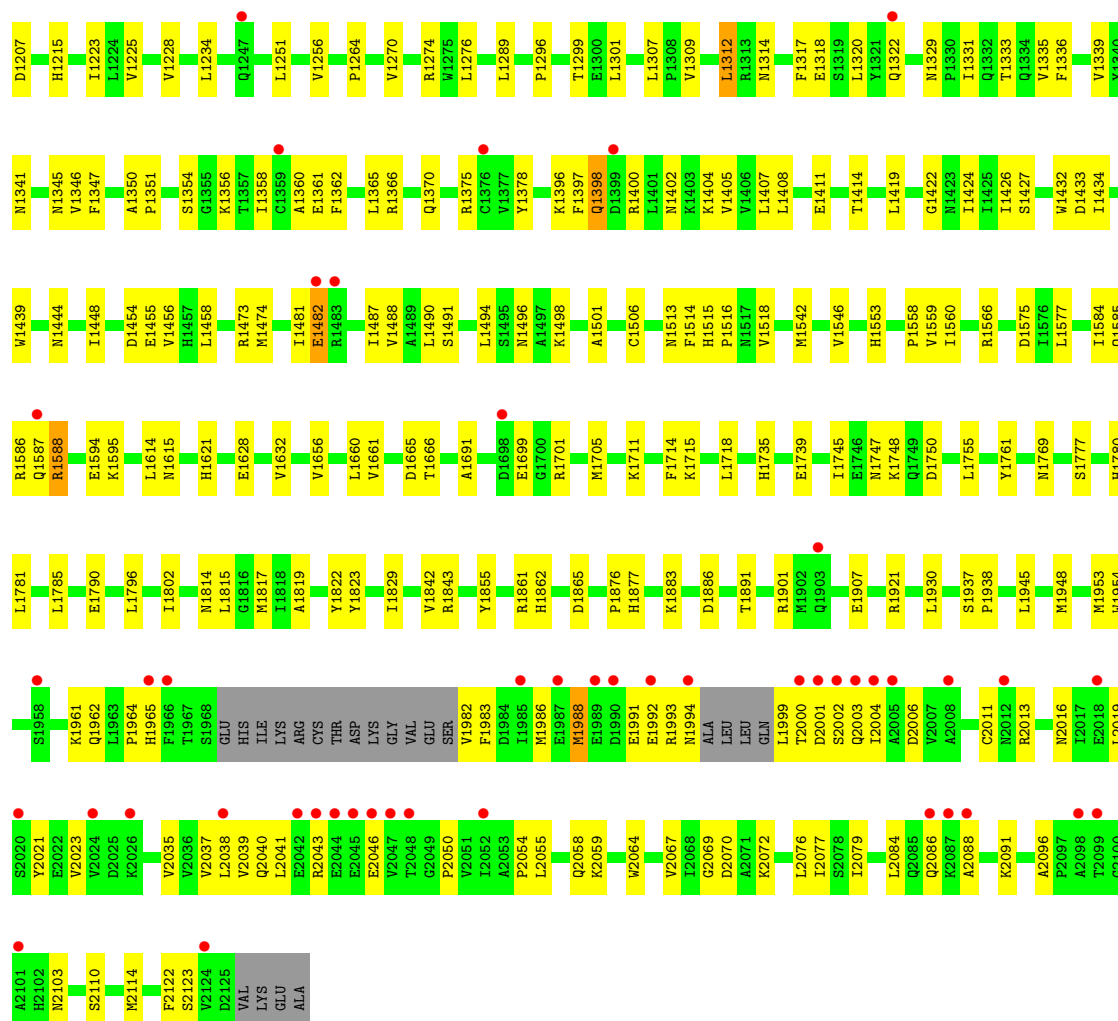
- Molecule 1: U5 small nuclear ribonucleoprotein 200 kDa helicase





• 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) 98.2 (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 0.214 , 0.260	Depositor DCC
R_{free} test set	6201 reflections (5.03%)	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 , 58.2	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	0.32	0/14095	0.55	3/19100 (0.0%)
1	B	0.31	0/13889	0.55	5/18815 (0.0%)
All	All	0.31	0/27984	0.55	8/37915 (0.0%)

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 (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	GLY	N-CA-C	-9.25	89.98	113.10
1	A	772	LEU	CA-CB-CG	6.37	129.96	115.30
1	A	821	LEU	CA-CB-CG	6.35	129.91	115.30
1	A	1312	LEU	CA-CB-CG	6.34	129.87	115.30
1	B	809	LEU	CA-CB-CG	5.86	128.78	115.30
1	B	772	LEU	CA-CB-CG	5.82	128.69	115.30
1	B	821	LEU	CA-CB-CG	5.26	127.40	115.30
1	B	1312	LEU	CA-CB-CG	5.12	127.08	115.30

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13802	0	13922	279	0
1	B	13603	0	13739	260	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	529	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 (529) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1814:ASN:HA	1:B:1817:MET:HE2	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:2501:8LV: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:1595:LYS:HZ2	1:B:666:ARG:HE	1.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1358:ILE:HA	1:A:1361:GLU:HB2	1.83	0.60
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:A:1814:ASN:HA	1:A:1817:MET:HE2	1.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:423:MET:HE2	1:B:425:ASN:HB3	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: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
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:2017:ILE:HD13	1:A:2108:PHE:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:SLV: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: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: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
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: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:A:988:ALA:HA	1:A:993:ILE:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:863:THR:HG22	1:B:864:LYS:N	2.27	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:754:GLU:C	1:A:756:SER:H	2.17	0.48
1:A:1741:VAL:HG13	1:A:1817:MET:HG2	1.95	0.48
1:B:933:PRO:HG3	1:B:943:LEU:HD22	1.95	0.48
1:B:1309:VAL:HB	1:B:1322:GLN:NE2	2.28	0.48
1:A:423:MET:HE2	1:A:425:ASN:HB3	1.95	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:1142:LYS:HE3	1:A:1146:LYS:HZ3	1.78	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1999:LEU:HD23	1:B:2000:THR:H	1.80	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:772:LEU:HG	1:A:773:GLU:HG3	1.96	0.47
1:A:1339:VAL:HA	1:A:1486:ARG:HH22	1.80	0.47
1:A:1870:GLN:O	1:A:1874:LYS:HG3	2.15	0.47
1:A:482:ASN:HB3	1:A:485:GLN:CD	2.36	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
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:A:1970:HIS:CG	1:A:1971:ILE:N	2.84	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1408:LEU:HD12	1:B:1427:SER:HB2	1.97	0.46
1:A:1501:ALA:HB1	1:A:1506:CYS:HB2	1.98	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
1:B:890:GLU:CD	1:B:928:ARG:HH21	2.20	0.45
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:B:767:GLU:O	1:B:770:LYS:NZ	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:1411:GLU:OE1	1:B:1414:THR:OG1	2.30	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: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:A:1539:LEU:HD22	1:A:1664:MET:HE3	2.00	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
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:1930:LEU:HD22	1:B:1938:PRO:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:784:ILE:HA	1:A:810:VAL:O	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1032:GLU:CD	1:A:1032:GLU:H	2.23	0.42
1:A:1093:ARG:HH21	1:A:1115:CYS:HB3	1.85	0.42
1:A:1482:GLU:CD	1:A:1482:GLU:H	2.23	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
1:A:654:THR:HG21	1:A:676:PHE:O	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1542:MET:HE2	1:B:1705:MET:HB3	2.01	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:1586:ARG:O	1:B:1587:GLN:HB2	2.20	0.41
1:B:1843:ARG:HH11	1:B:1877:HIS:CE1	2.39	0.41
1:A:1276:LEU:HD23	1:A:1276:LEU:HA	1.95	0.41
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: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: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:509:LYS:H	1:A:509:LYS:HG2	1.68	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:1433:ASP:OD1	1:B:1823:TYR:OH	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:2068:ILE:HG22	1:A:2077:ILE:HB	2.02	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: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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	34	66
1	B	1677/1738 (96%)	1603 (96%)	70 (4%)	4 (0%)	47	78
All	All	3391/3476 (98%)	3236 (95%)	145 (4%)	10 (0%)	41	72

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%)	1509 (98%)	25 (2%)	62	88
1	B	1514/1551 (98%)	1493 (99%)	21 (1%)	67	90
All	All	3048/3102 (98%)	3002 (98%)	46 (2%)	65	89

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	462	LEU
1	A	489	TYR

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Mol	Chain	Res	Type
1	A	526	ASN
1	A	545	ARG
1	A	546	SER
1	A	602	GLU
1	A	610	ARG
1	A	756	SER
1	A	759	THR
1	A	760	GLU
1	A	875	GLU
1	A	876	LEU
1	A	877	GLN
1	A	992	TYR
1	A	1307	LEU
1	A	1575	ASP
1	A	1588	ARG
1	A	1656	VAL
1	A	1699	GLU
1	A	1731	CYS
1	A	1842	VAL
1	A	1862	HIS
1	A	1973	ARG
1	A	2000	THR
1	A	2023	VAL
1	B	426	LYS
1	B	462	LEU
1	B	489	TYR
1	B	546	SER
1	B	602	GLU
1	B	610	ARG
1	B	770	LYS
1	B	778	LEU
1	B	792	VAL
1	B	809	LEU
1	B	939	SER
1	B	1016	ARG
1	B	1093	ARG
1	B	1170	MET
1	B	1398	GLN
1	B	1575	ASP
1	B	1588	ARG
1	B	1699	GLU
1	B	1842	VAL

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Mol	Chain	Res	Type
1	B	1862	HIS
1	B	2084	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	GLN
1	A	526	ASN
1	A	532	ASN
1	A	1690	HIS
1	A	2040	GLN
1	A	2118	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	29,36,36	1.36	3 (10%)	28,52,52	1.54	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	8LV	B	2501	-	29,36,36	1.54	3 (10%)	28,52,52	1.47	4 (14%)

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	-	-	4/8/32/32	0/5/5/5
2	8LV	B	2501	-	-	2/8/32/32	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2501	8LV	C14-C13	-4.71	1.48	1.51
2	B	2501	8LV	C16-C15	4.08	1.49	1.45
2	A	2501	8LV	C16-C15	3.98	1.49	1.45
2	A	2501	8LV	C14-C13	-3.35	1.49	1.51
2	B	2501	8LV	C24-C15	-3.34	1.34	1.38
2	A	2501	8LV	C24-C15	-3.08	1.34	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2501	8LV	C15-C24-N25	-4.41	119.16	123.57
2	B	2501	8LV	C15-C24-N25	-4.24	119.33	123.57
2	A	2501	8LV	C14-C15-C16	3.29	122.97	117.26
2	B	2501	8LV	C7-C8-C10	-3.06	116.55	120.42
2	B	2501	8LV	C14-C15-C16	2.69	121.93	117.26
2	A	2501	8LV	C7-C8-C10	-2.53	117.23	120.42
2	A	2501	8LV	C9-C8-C10	2.50	123.58	120.42
2	B	2501	8LV	C9-C8-C10	2.27	123.30	120.42

There are no chirality outliers.

All (6) 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

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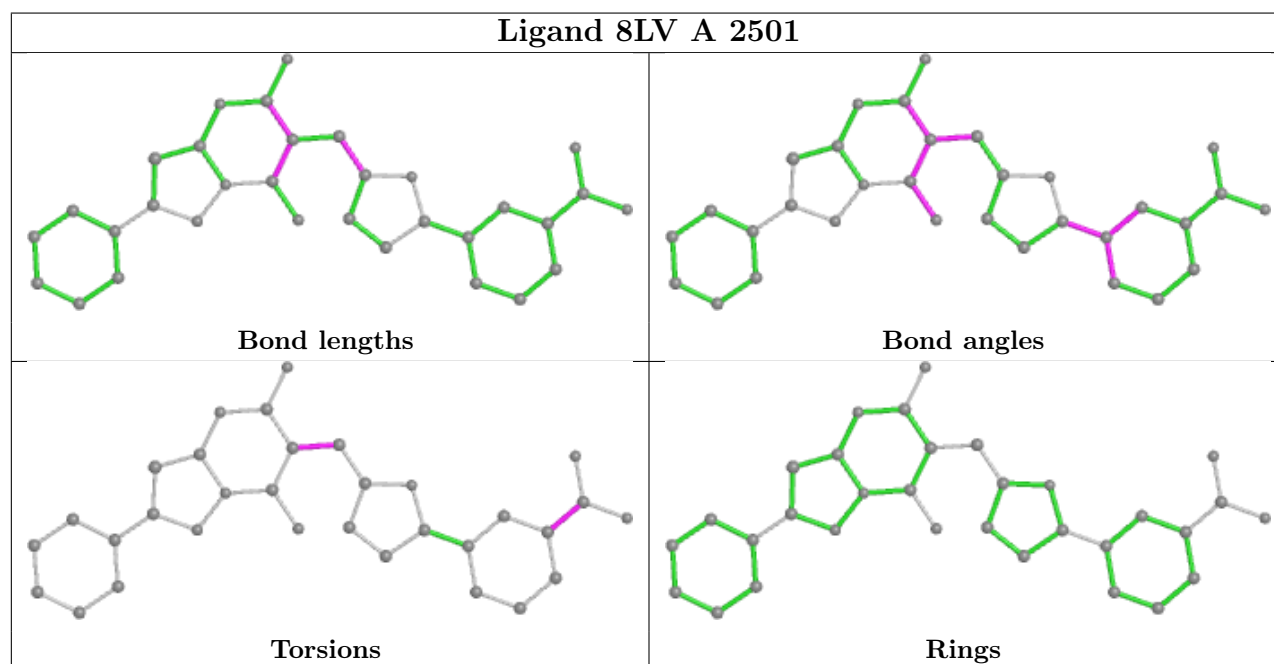
Mol	Chain	Res	Type	Atoms
2	B	2501	8LV	C13-C14-C15-C16
2	A	2501	8LV	O3-C2-C4-C9
2	A	2501	8LV	O3-C2-C4-C5

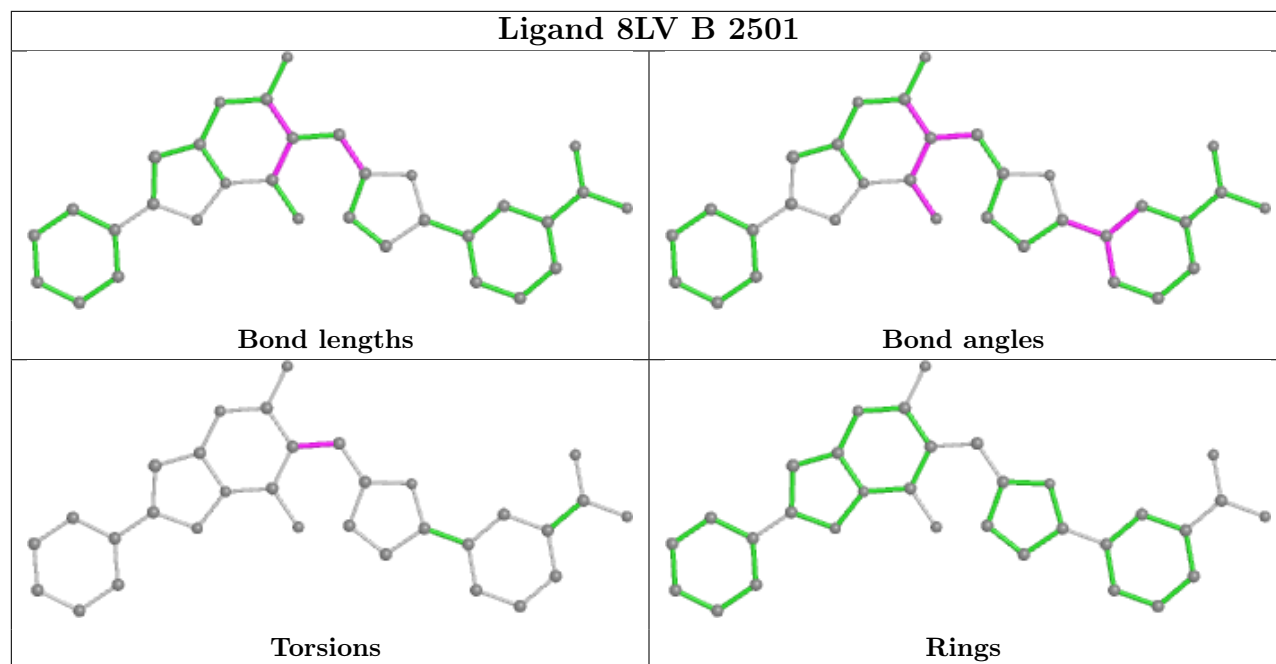
There are no ring outliers.

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1718/1738 (98%)	0.05	100 (5%) 23 15	41, 71, 126, 176	0
1	B	1691/1738 (97%)	0.10	86 (5%) 28 19	46, 76, 122, 160	0
All	All	3409/3476 (98%)	0.07	186 (5%) 25 16	41, 74, 123, 176	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1975	THR	10.0
1	B	1990	ASP	7.5
1	A	1994	ASN	7.4
1	A	745	LYS	7.3
1	A	1995	ALA	6.7
1	B	747	THR	6.3
1	B	746	ASP	6.3
1	A	1974	CYS	6.2
1	A	2088	ALA	5.9
1	A	746	ASP	5.9
1	B	751	PHE	5.8
1	A	2004	ILE	5.8
1	A	2003	GLN	5.6
1	B	2042	GLU	5.4
1	B	2004	ILE	5.4
1	A	2042	GLU	5.4
1	A	1980	GLU	5.3
1	B	2005	ALA	5.3
1	B	2099	THR	5.2
1	B	1050	GLU	5.2
1	A	530	THR	5.2
1	A	2048	THR	5.2
1	B	457	SER	5.1
1	B	2003	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	758	SER	4.9
1	A	694	GLU	4.8
1	A	1969	GLU	4.8
1	A	1996	LEU	4.5
1	A	2005	ALA	4.5
1	B	2020	SER	4.5
1	A	527	MET	4.4
1	A	2044	GLU	4.4
1	B	863	THR	4.3
1	A	1988	MET	4.3
1	A	1968	SER	4.3
1	A	528	ASP	4.3
1	A	1050	GLU	4.3
1	B	2101	ALA	4.3
1	A	1587	GLN	4.3
1	B	754	GLU	4.2
1	B	2001	ASP	4.2
1	B	1587	GLN	4.2
1	A	2047	VAL	4.1
1	A	2087	LYS	4.1
1	A	1992	GLU	4.0
1	B	527	MET	4.0
1	A	1984	ASP	4.0
1	B	2087	LYS	3.9
1	B	530	THR	3.9
1	B	1994	ASN	3.9
1	A	1997	LEU	3.8
1	A	529	GLY	3.8
1	B	526	ASN	3.7
1	A	695	LYS	3.7
1	A	2124	VAL	3.7
1	A	2098	ALA	3.7
1	A	941	ASP	3.6
1	B	2098	ALA	3.6
1	B	432	ASP	3.6
1	B	437	ARG	3.6
1	A	516	CYS	3.6
1	B	2048	THR	3.5
1	A	747	THR	3.5
1	A	2012	ASN	3.5
1	B	2046	GLU	3.5
1	B	698	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1983	PHE	3.5
1	A	2008	ALA	3.5
1	A	1987	GLU	3.4
1	B	745	LYS	3.4
1	B	1989	GLU	3.4
1	B	454	PRO	3.4
1	B	2045	GLU	3.4
1	A	1990	ASP	3.4
1	B	2000	THR	3.4
1	A	437	ARG	3.3
1	B	2086	GLN	3.3
1	B	860	GLN	3.2
1	B	1247	GLN	3.2
1	A	2059	LYS	3.2
1	A	2101	ALA	3.2
1	B	2047	VAL	3.1
1	B	2052	ILE	3.1
1	B	697	ALA	3.1
1	A	1991	GLU	3.1
1	A	1981	SER	3.0
1	A	1998	GLN	3.0
1	B	574	GLN	3.0
1	B	974	LYS	3.0
1	B	1138	GLU	3.0
1	B	453	LYS	2.9
1	B	696	LYS	2.9
1	A	2045	GLU	2.9
1	B	861	TYR	2.9
1	A	1903	GLN	2.9
1	A	741	MET	2.9
1	A	2018	GLU	2.9
1	B	1137	GLU	2.8
1	B	1399	ASP	2.8
1	A	1147	ASN	2.8
1	A	2040	GLN	2.8
1	A	2086	GLN	2.8
1	A	2125	ASP	2.8
1	A	2043	ARG	2.8
1	A	2099	THR	2.8
1	A	2052	ILE	2.7
1	A	2009	ARG	2.7
1	B	2088	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	2124	VAL	2.7
1	A	2089	LYS	2.7
1	A	1985	ILE	2.7
1	A	2027	ASP	2.7
1	B	528	ASP	2.7
1	B	1147	ASN	2.6
1	B	2012	ASN	2.6
1	A	748	LEU	2.6
1	B	2038	LEU	2.6
1	B	1482	GLU	2.6
1	B	2002	SER	2.6
1	A	405	PRO	2.6
1	B	1966	PHE	2.6
1	B	569	LEU	2.5
1	B	1987	GLU	2.5
1	A	2024	VAL	2.5
1	B	405	PRO	2.5
1	B	441	GLY	2.5
1	B	2043	ARG	2.5
1	A	1870	GLN	2.5
1	A	744	GLU	2.5
1	B	426	LYS	2.5
1	B	456	GLY	2.5
1	A	1972	LYS	2.5
1	A	2102	HIS	2.5
1	B	1322	GLN	2.5
1	A	792	VAL	2.4
1	A	526	ASN	2.4
1	A	2001	ASP	2.4
1	B	1958	SER	2.4
1	A	476	GLU	2.4
1	A	1228	VAL	2.4
1	B	478	PHE	2.4
1	A	1247	GLN	2.4
1	A	1260	GLU	2.4
1	A	2002	SER	2.4
1	B	1903	GLN	2.4
1	A	2071	ALA	2.4
1	B	1359	CYS	2.4
1	A	1967	THR	2.4
1	B	2044	GLU	2.3
1	A	1999	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	573	HIS	2.3
1	B	694	GLU	2.3
1	A	751	PHE	2.3
1	B	1376	CYS	2.3
1	A	1989	GLU	2.3
1	A	432	ASP	2.2
1	A	1956	LYS	2.2
1	B	1992	GLU	2.2
1	A	940	HIS	2.2
1	A	1695	LEU	2.2
1	A	939	SER	2.2
1	B	2024	VAL	2.2
1	A	2041	LEU	2.2
1	B	2018	GLU	2.2
1	A	2046	GLU	2.2
1	A	477	GLY	2.2
1	B	1985	ILE	2.2
1	A	1970	HIS	2.2
1	B	529	GLY	2.1
1	A	1874	LYS	2.1
1	A	427	ARG	2.1
1	B	1965	HIS	2.1
1	B	1072	LEU	2.1
1	A	1993	ARG	2.1
1	A	757	ALA	2.1
1	B	433	GLY	2.1
1	B	455	PHE	2.1
1	B	1698	ASP	2.1
1	A	975	LYS	2.1
1	A	1966	PHE	2.1
1	B	2026	LYS	2.1
1	B	429	GLN	2.1
1	B	2008	ALA	2.1
1	A	513	ALA	2.0
1	B	1483	ARG	2.0
1	A	755	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

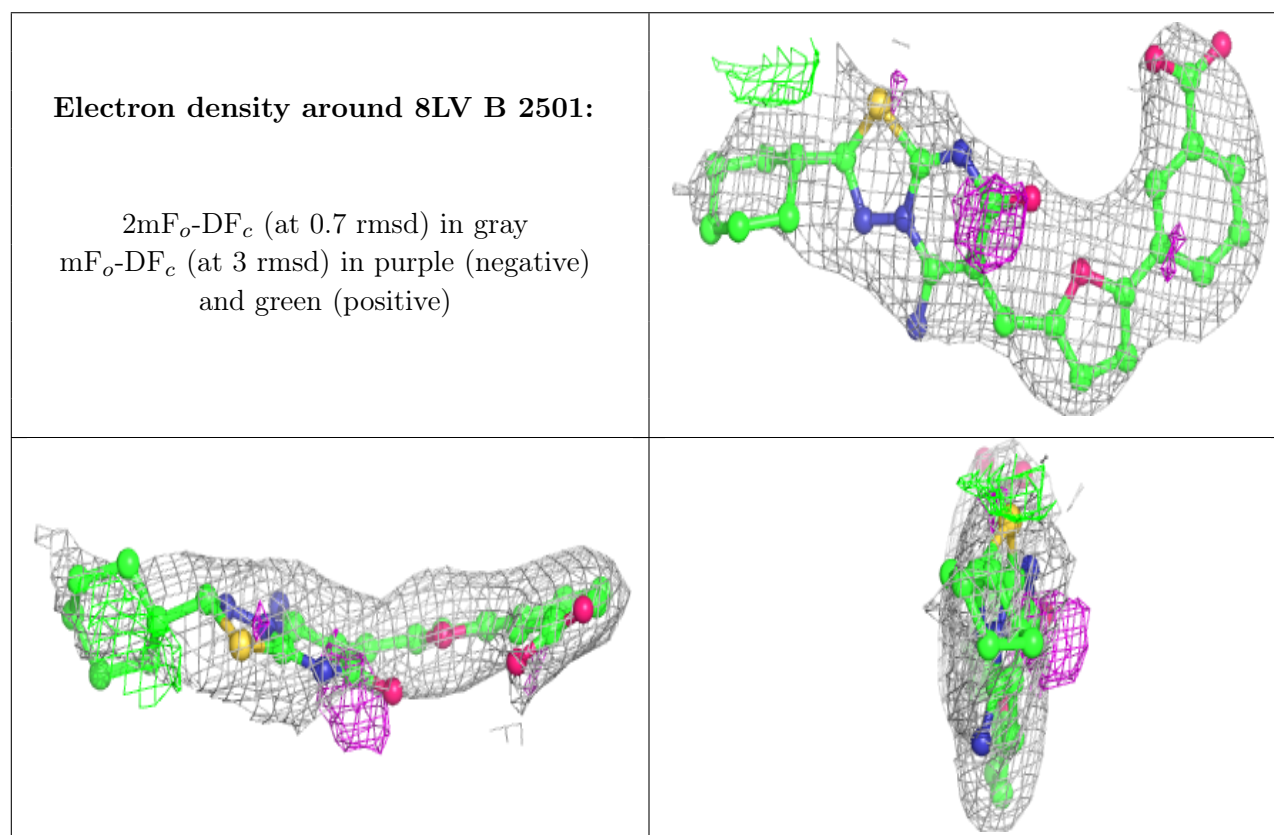
There are no monosaccharides in this entry.

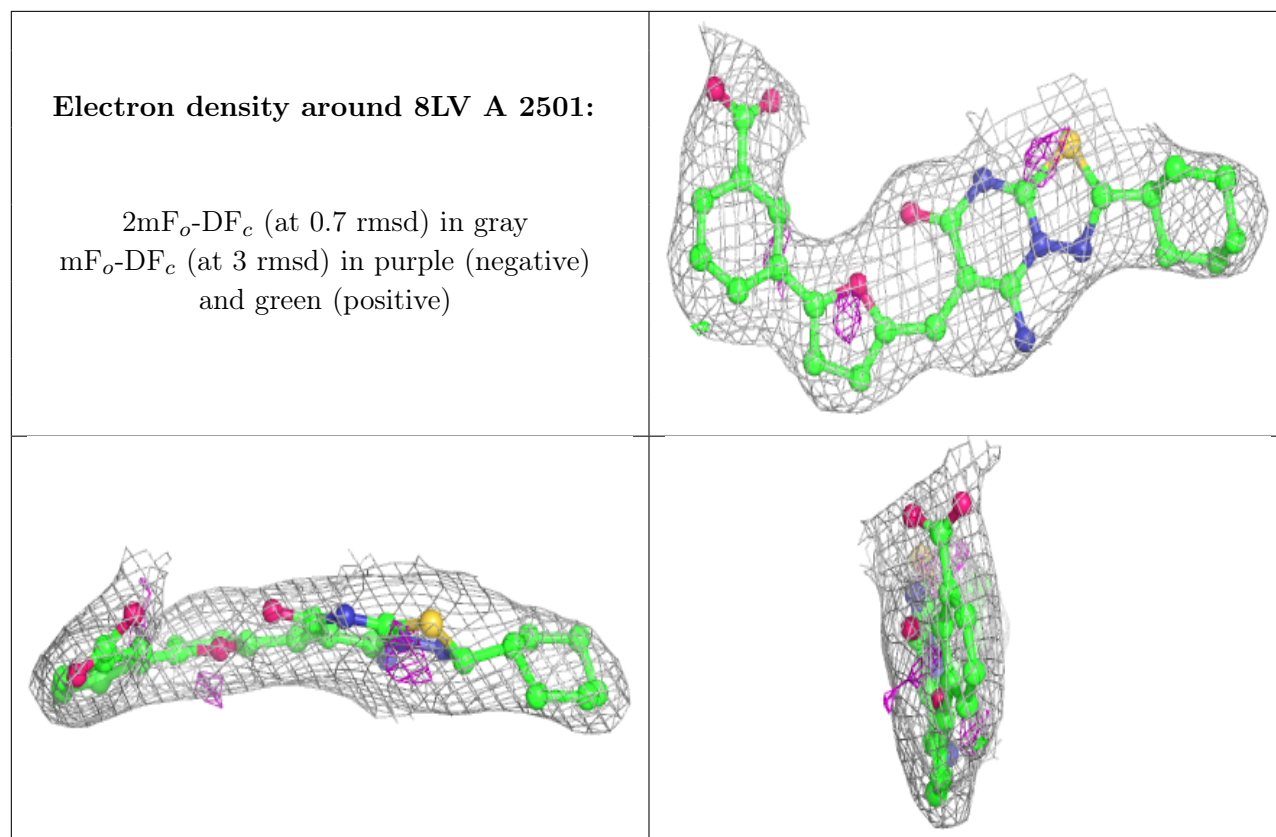
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	8LV	B	2501	32/32	0.86	0.27	64,88,112,117	0
2	8LV	A	2501	32/32	0.90	0.21	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.