



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2023 – 12:20 pm GMT

PDB ID : 8BCH
Title : Human Brr2 Helicase Region in complex with Sulfaguanidine
Authors : Vester, K.; Loll, B.; Wahl, M.C.
Deposited on : 2022-10-15
Resolution : 2.87 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.32.1
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) : 2.32.1

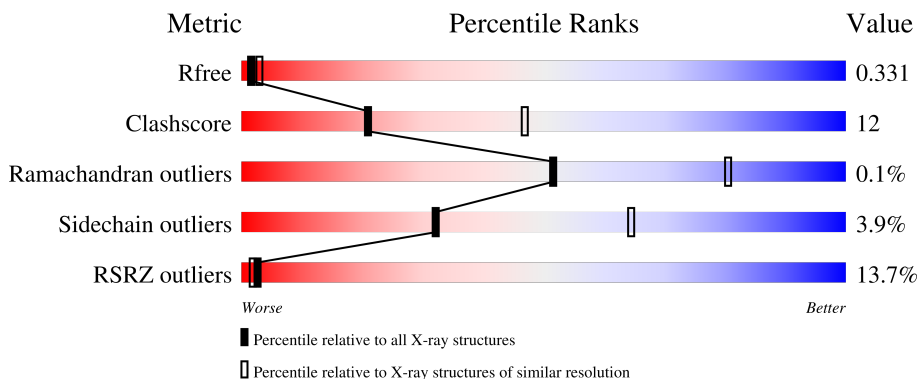
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

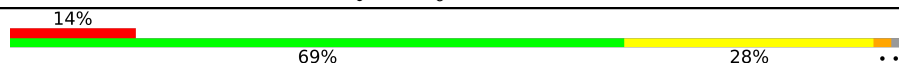
The reported resolution of this entry is 2.87 Å.

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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	B	1747	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 13884 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.

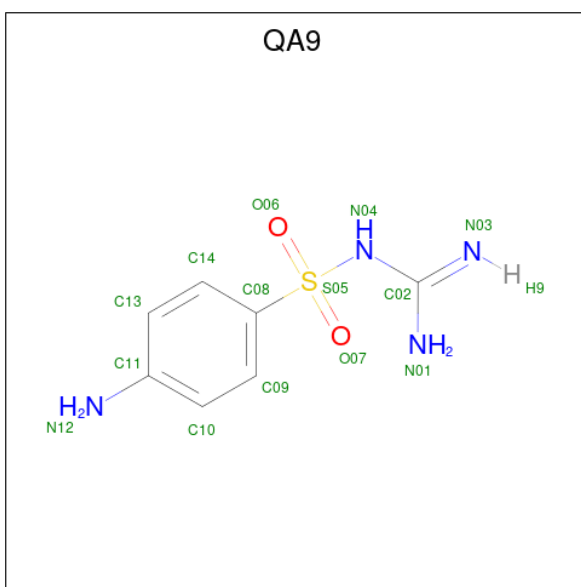
- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	1724	13859	8857	2371	2559	72	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	390	GLY	-	expression tag	UNP O75643
B	391	ALA	-	expression tag	UNP O75643
B	392	GLU	-	expression tag	UNP O75643
B	393	PHE	-	expression tag	UNP O75643

- Molecule 2 is 1-(4-aminophenyl)sulfonylguanidine (three-letter code: QA9) (formula: C₇H₁₀N₄O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	14	7	4	2	1	0	0

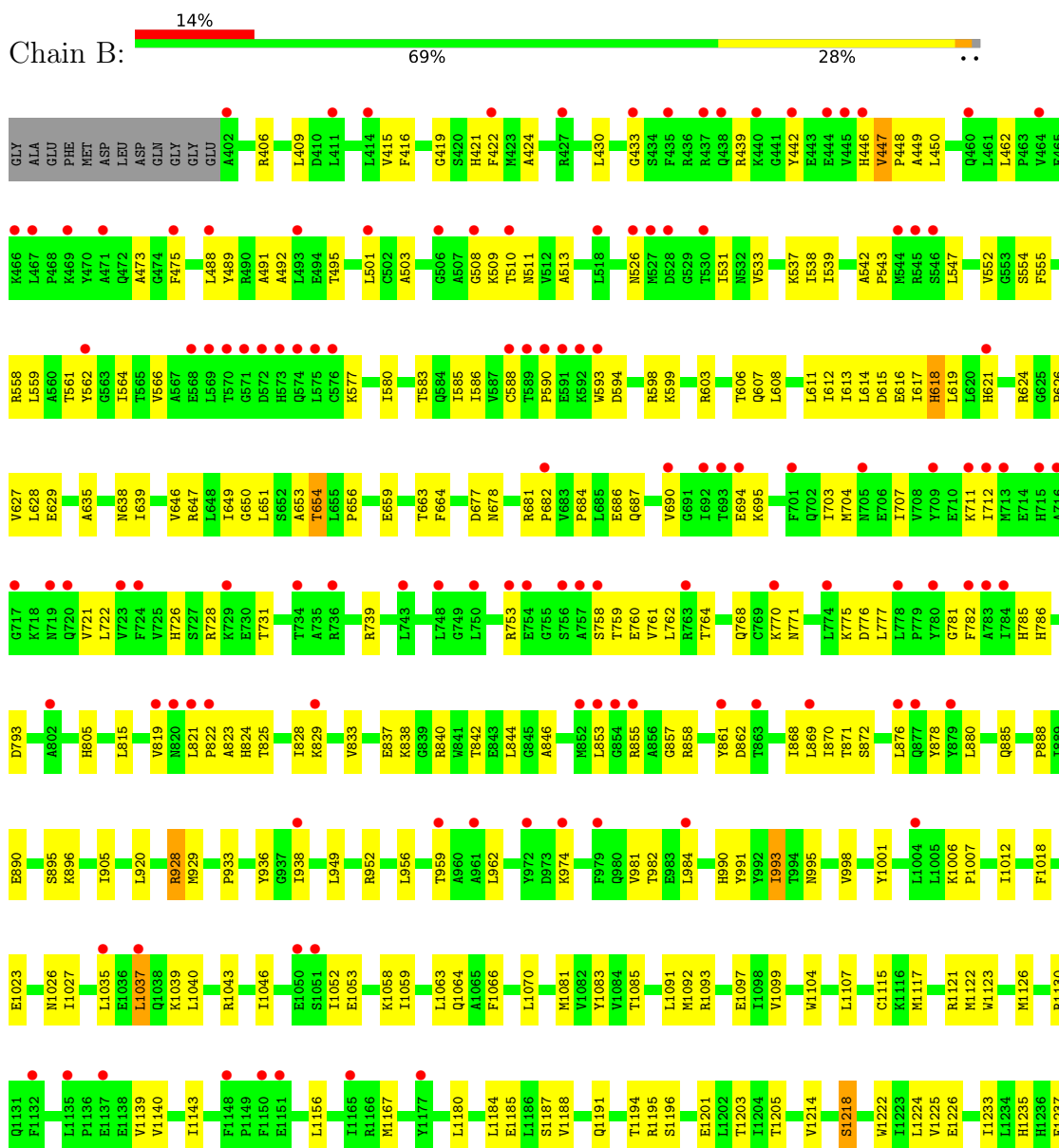
- Molecule 3 is water.

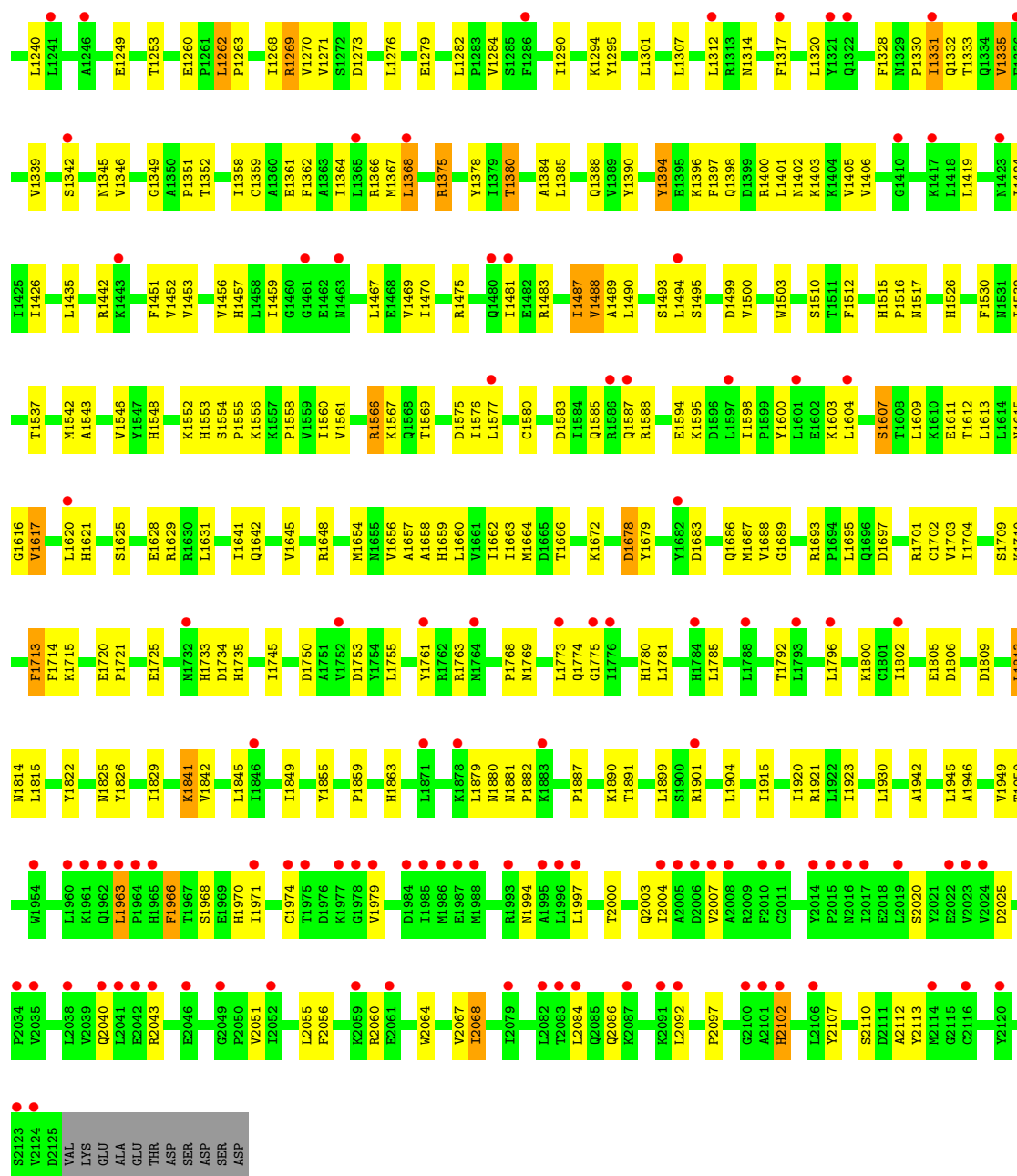
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	11	Total O 11 11	0	0

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





4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.29Å 149.53Å 141.49Å 90.00° 120.32° 90.00°	Depositor
Resolution (Å)	47.20 – 2.87 47.20 – 2.87	Depositor EDS
% Data completeness (in resolution range)	93.2 (47.20-2.87) 93.3 (47.20-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.281 , 0.337 0.278 , 0.331	Depositor DCC
R_{free} test set	2013 reflections (3.58%)	wwPDB-VP
Wilson B-factor (Å ²)	82.8	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-1/2*h-1/2*k-l 0.000 for -k,-h,-1/2*h+1/2*k-l 0.001 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13884	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: QA9

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	B	0.26	0/14153	0.50	0/19177

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	13859	0	14001	341	0
2	B	14	0	0	0	0
3	B	11	0	0	0	0
All	All	13884	0	14001	341	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 12.

All (341) 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:415:VAL:HG21	1:B:895:SER:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ARG:NH2	1:B:974:LYS:O	2.19	0.74
1:B:1950:THR:HG22	1:B:2060:ARG:HH12	1.52	0.74
1:B:1526:HIS:HB2	1:B:1703:VAL:HG12	1.69	0.74
1:B:1710:LYS:O	1:B:1713:PHE:HB3	1.88	0.73
1:B:1378:TYR:HB3	1:B:1426:ILE:HG22	1.71	0.73
1:B:1328:PHE:HB3	1:B:1332:GLN:HG3	1.70	0.72
1:B:492:ALA:HA	1:B:647:ARG:HH22	1.53	0.72
1:B:1950:THR:HG21	1:B:2112:ALA:HA	1.72	0.72
1:B:626:PRO:HG2	1:B:896:LYS:HG3	1.72	0.71
1:B:1974:CYS:HB3	1:B:1979:VAL:HB	1.74	0.70
1:B:1320:LEU:HG	1:B:1396:LYS:HD3	1.72	0.70
1:B:1405:VAL:HG22	1:B:1424:ILE:HB	1.74	0.69
1:B:1734:ASP:OD2	1:B:1825:ASN:ND2	2.22	0.69
1:B:531:ILE:HD13	1:B:533:VAL:HG13	1.75	0.68
1:B:1577:LEU:HD11	1:B:1615:ASN:HB3	1.73	0.68
1:B:1800:LYS:HB2	1:B:1815:LEU:HD12	1.76	0.68
1:B:1345:ASN:HB3	1:B:1487:ILE:HG22	1.76	0.68
1:B:1966:PHE:HE1	1:B:1970:HIS:HB2	1.58	0.68
1:B:753:ARG:HD2	1:B:760:GLU:HB2	1.75	0.67
1:B:758:SER:OG	1:B:759:THR:N	2.27	0.67
1:B:1027:ILE:HG21	1:B:1059:ILE:HD11	1.77	0.67
1:B:566:VAL:HG12	1:B:585:ILE:HB	1.77	0.66
1:B:1301:LEU:HD21	1:B:1330:PRO:HB2	1.76	0.66
1:B:1359:CYS:O	1:B:1362:PHE:HB2	1.96	0.66
1:B:1301:LEU:HD22	1:B:1331:ILE:HG22	1.76	0.66
1:B:1660:LEU:HA	1:B:1701:ARG:O	1.97	0.65
1:B:2051:VAL:HG13	1:B:2113:TYR:HE1	1.60	0.65
1:B:1185:GLU:HB2	1:B:1205:THR:HB	1.78	0.65
1:B:1390:TYR:HB2	1:B:1426:ILE:HD11	1.77	0.65
1:B:993:ILE:HD11	1:B:998:VAL:HG23	1.78	0.65
1:B:1225:VAL:HG22	1:B:1268:ILE:HG22	1.78	0.65
1:B:768:GLN:HE21	1:B:775:LYS:HA	1.60	0.65
1:B:690:VAL:HG22	1:B:870:ILE:HA	1.79	0.64
1:B:678:ASN:OD1	1:B:885:GLN:NE2	2.31	0.64
1:B:758:SER:HB2	1:B:762:LEU:HB2	1.80	0.64
1:B:1226:GLU:OE2	1:B:1269:ARG:NH1	2.31	0.64
1:B:1222:TRP:NE1	1:B:1273:ASP:OD2	2.30	0.63
1:B:991:TYR:HE2	1:B:1097:GLU:HG3	1.63	0.63
1:B:1585:GLN:HB3	1:B:1588:ARG:HB2	1.81	0.63
1:B:777:LEU:HB3	1:B:782:PHE:HB2	1.81	0.62
1:B:539:ILE:HG22	1:B:586:ILE:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1456:VAL:HG21	1:B:1489:ALA:HB1	1.81	0.62
1:B:659:GLU:O	1:B:663:THR:HG23	2.00	0.62
1:B:1339:VAL:HG22	1:B:1346:VAL:HG21	1.80	0.62
1:B:929:MET:HE2	1:B:949:LEU:HD13	1.82	0.62
1:B:1081:MET:O	1:B:1085:THR:HG23	2.00	0.61
1:B:858:ARG:HE	1:B:861:TYR:HB2	1.65	0.61
1:B:858:ARG:N	1:B:862:ASP:OD2	2.31	0.61
1:B:543:PRO:HD2	1:B:547:LEU:HD23	1.83	0.61
1:B:753:ARG:HH21	1:B:761:VAL:HG22	1.66	0.61
1:B:1195:ARG:NH1	1:B:1260:GLU:OE2	2.32	0.61
1:B:2043:ARG:HB3	1:B:2086:GLN:HA	1.83	0.60
1:B:419:GLY:O	1:B:421:HIS:N	2.32	0.60
1:B:1859:PRO:O	1:B:1890:LYS:NZ	2.31	0.60
1:B:1966:PHE:CE1	1:B:1970:HIS:HB2	2.37	0.59
1:B:537:LYS:NZ	1:B:583:THR:O	2.36	0.59
1:B:1451:PHE:HB3	1:B:1487:ILE:HD12	1.84	0.58
1:B:488:LEU:HD21	1:B:501:LEU:HD13	1.86	0.58
1:B:656:PRO:HG2	1:B:888:PRO:HA	1.84	0.58
1:B:768:GLN:NE2	1:B:775:LYS:HA	2.18	0.58
1:B:555:PHE:O	1:B:559:LEU:HG	2.03	0.58
1:B:2043:ARG:HH21	1:B:2084:LEU:HD23	1.68	0.58
1:B:508:GLY:O	1:B:510:THR:N	2.35	0.57
1:B:984:LEU:HD12	1:B:998:VAL:HG13	1.84	0.57
1:B:619:LEU:HD11	1:B:624:ARG:HB2	1.85	0.57
1:B:712:ILE:HG12	1:B:721:VAL:HB	1.87	0.57
1:B:982:THR:HG22	1:B:984:LEU:H	1.69	0.57
1:B:1066:PHE:O	1:B:1121:ARG:NH1	2.36	0.57
1:B:1368:LEU:HD21	1:B:1403:LYS:HE2	1.86	0.57
1:B:1842:VAL:HA	1:B:1845:LEU:HD22	1.87	0.57
1:B:552:VAL:HG23	1:B:566:VAL:HG23	1.87	0.57
1:B:1312:LEU:HD21	1:B:1317:PHE:HB3	1.87	0.56
1:B:1235:HIS:NE2	1:B:1237:GLU:HG3	2.21	0.56
1:B:1994:ASN:HA	1:B:1997:LEU:HD12	1.88	0.56
1:B:1364:ILE:O	1:B:1367:MET:HB3	2.05	0.56
1:B:1397:PHE:O	1:B:1402:ASN:N	2.39	0.56
1:B:1595:LYS:HD3	1:B:1598:ILE:HD12	1.87	0.56
1:B:694:GLU:HG2	1:B:695:LYS:H	1.71	0.55
1:B:1500:VAL:HG23	1:B:1503:TRP:HE3	1.69	0.55
1:B:1575:ASP:OD1	1:B:1576:ILE:N	2.40	0.55
1:B:1099:VAL:HG21	1:B:1107:LEU:HB3	1.88	0.55
1:B:1920:ILE:HA	1:B:1923:ILE:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.88	0.54
1:B:929:MET:HE3	1:B:938:ILE:HD11	1.89	0.54
1:B:1130:ARG:HG2	1:B:1140:VAL:HG11	1.88	0.54
1:B:1368:LEU:HD11	1:B:1403:LYS:HG2	1.88	0.54
1:B:824:HIS:ND1	1:B:862:ASP:OD1	2.40	0.54
1:B:424:ALA:HB3	1:B:888:PRO:HG2	1.88	0.54
1:B:1566:ARG:HB2	1:B:1621:HIS:HB2	1.90	0.54
1:B:1332:GLN:HA	1:B:1335:VAL:HG12	1.89	0.54
1:B:1384:ALA:O	1:B:1388:GLN:HG2	2.08	0.54
1:B:1092:MET:HB3	1:B:1115:CYS:SG	2.47	0.53
1:B:1018:PHE:CE2	1:B:1063:LEU:HD22	2.43	0.53
1:B:447:VAL:HG22	1:B:687:GLN:HG3	1.91	0.53
1:B:1688:VAL:HG22	1:B:1702:CYS:SG	2.49	0.53
1:B:539:ILE:HD11	1:B:612:ILE:HG23	1.91	0.53
1:B:677:ASP:HB2	1:B:885:GLN:HE22	1.73	0.53
1:B:1035:LEU:O	1:B:1039:LYS:HG2	2.09	0.53
1:B:728:ARG:HG2	1:B:786:HIS:CG	2.44	0.52
1:B:1543:ALA:O	1:B:1546:VAL:HG22	2.10	0.52
1:B:1733:HIS:CD2	1:B:1792:THR:HG22	2.44	0.52
1:B:1813:LEU:HD22	1:B:1814:ASN:H	1.74	0.52
1:B:1997:LEU:HD13	1:B:2004:ILE:HG22	1.92	0.52
1:B:491:ALA:O	1:B:495:THR:OG1	2.19	0.52
1:B:513:ALA:HB1	1:B:613:ILE:HD13	1.90	0.52
1:B:538:ILE:O	1:B:585:ILE:HA	2.10	0.52
1:B:1845:LEU:HB3	1:B:1945:LEU:HD22	1.90	0.52
1:B:933:PRO:HB2	1:B:938:ILE:HB	1.92	0.52
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.91	0.52
1:B:1612:THR:OG1	1:B:1617:VAL:HG13	2.09	0.52
1:B:635:ALA:O	1:B:639:ILE:HG23	2.10	0.52
1:B:1453:VAL:HG22	1:B:1456:VAL:HG22	1.92	0.52
1:B:473:ALA:HB3	1:B:562:TYR:CZ	2.45	0.51
1:B:823:ALA:O	1:B:857:GLY:N	2.40	0.51
1:B:1946:ALA:O	1:B:1950:THR:HG23	2.11	0.51
1:B:1290:ILE:HD13	1:B:1768:PRO:HD2	1.92	0.51
1:B:1335:VAL:HG23	1:B:1512:PHE:CD2	2.45	0.51
1:B:1218:SER:HB2	1:B:1240:LEU:HD21	1.93	0.51
1:B:1796:LEU:HB3	1:B:1802:ILE:HG23	1.93	0.51
1:B:1188:VAL:HG11	1:B:1284:VAL:HG12	1.92	0.51
1:B:614:LEU:HD23	1:B:628:LEU:HD22	1.92	0.51
1:B:446:HIS:NE2	1:B:686:GLU:HG2	2.25	0.51
1:B:1625:SER:HB2	1:B:1628:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ILE:HD11	1:B:612:ILE:HG12	1.93	0.51
1:B:704:MET:HE3	1:B:829:LYS:HG2	1.93	0.51
1:B:442:TYR:HE1	1:B:707:ILE:HG12	1.76	0.51
1:B:611:LEU:HD11	1:B:649:ILE:HG12	1.93	0.50
1:B:1560:ILE:HD11	1:B:1656:VAL:HG12	1.92	0.50
1:B:711:LYS:HG3	1:B:868:ILE:HD13	1.93	0.50
1:B:681:ARG:HG3	1:B:682:PRO:HD2	1.93	0.50
1:B:1553:HIS:O	1:B:1701:ARG:NH1	2.44	0.50
1:B:629:GLU:HA	1:B:664:PHE:HZ	1.76	0.50
1:B:503:ALA:HB3	1:B:509:LYS:HD3	1.94	0.50
1:B:1349:GLY:N	1:B:1512:PHE:O	2.32	0.50
1:B:1001:TYR:OH	1:B:1091:LEU:HD12	2.12	0.49
1:B:603:ARG:NH2	1:B:607:GLN:HA	2.27	0.49
1:B:722:LEU:HD22	1:B:823:ALA:HB2	1.94	0.49
1:B:1678:ASP:OD1	1:B:1710:LYS:NZ	2.40	0.49
1:B:599:LYS:HA	1:B:990:HIS:CD2	2.48	0.49
1:B:1314:ASN:HB3	1:B:1317:PHE:HB2	1.95	0.49
1:B:1585:GLN:O	1:B:1587:GLN:N	2.42	0.49
1:B:2068:ILE:HD11	1:B:2092:LEU:HD13	1.95	0.49
1:B:1307:LEU:HG	1:B:1333:THR:HG23	1.95	0.49
1:B:768:GLN:HB3	1:B:775:LYS:NZ	2.28	0.49
1:B:2020:SER:OG	1:B:2040:GLN:HB2	2.13	0.49
1:B:1352:THR:HG22	1:B:1689:GLY:HA3	1.95	0.48
1:B:1566:ARG:HG3	1:B:1567:LYS:H	1.78	0.48
1:B:1364:ILE:HG21	1:B:1424:ILE:HD11	1.94	0.48
1:B:1515:HIS:ND1	1:B:1516:PRO:HD2	2.29	0.48
1:B:449:ALA:HB1	1:B:684:PRO:HB2	1.95	0.48
1:B:1271:VAL:HG13	1:B:1279:GLU:HB2	1.94	0.48
1:B:1046:ILE:HB	1:B:1064:GLN:NE2	2.28	0.48
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.53	0.48
1:B:1194:THR:HG23	1:B:1196:SER:H	1.78	0.48
1:B:1620:LEU:HD22	1:B:1629:ARG:HG2	1.95	0.48
1:B:1469:VAL:HG21	1:B:1735:HIS:NE2	2.28	0.48
1:B:1604:LEU:HD21	1:B:1631:LEU:HD23	1.95	0.48
1:B:1346:VAL:HA	1:B:1510:SER:HB3	1.96	0.48
1:B:1775:GLY:HA3	1:B:1780:HIS:CG	2.49	0.47
1:B:433:GLY:O	1:B:448:PRO:HD3	2.15	0.47
1:B:1664:MET:O	1:B:1666:THR:N	2.41	0.47
1:B:838:LYS:HB3	1:B:840:ARG:HG2	1.96	0.47
1:B:1663:ILE:HD12	1:B:1704:ILE:HG12	1.96	0.47
1:B:1725:GLU:OE2	1:B:1763:ARG:NH2	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1139:VAL:O	1:B:1143:ILE:HG13	2.14	0.47
1:B:1295:TYR:CG	1:B:1495:SER:HB2	2.48	0.47
1:B:871:THR:OG1	1:B:872:SER:N	2.48	0.47
1:B:2064:TRP:CZ3	1:B:2110:SER:HB3	2.50	0.47
1:B:450:LEU:HD12	1:B:678:ASN:HB2	1.96	0.47
1:B:928:ARG:HD2	1:B:928:ARG:HA	1.71	0.47
1:B:599:LYS:HA	1:B:990:HIS:HD2	1.80	0.47
1:B:837:GLU:HG3	1:B:1083:TYR:CE1	2.49	0.47
1:B:1224:LEU:HD23	1:B:1233:ILE:HD13	1.96	0.46
1:B:1452:VAL:HA	1:B:1488:VAL:O	2.15	0.46
1:B:776:ASP:OD1	1:B:777:LEU:N	2.48	0.46
1:B:1290:ILE:HG13	1:B:1769:ASN:OD1	2.14	0.46
1:B:678:ASN:ND2	1:B:681:ARG:HH21	2.13	0.46
1:B:538:ILE:HB	1:B:585:ILE:HG12	1.98	0.46
1:B:876:LEU:O	1:B:880:LEU:HG	2.15	0.46
1:B:1352:THR:HG21	1:B:1686:GLN:HA	1.97	0.46
1:B:1855:TYR:HB3	1:B:1891:THR:HG21	1.98	0.46
1:B:639:ILE:HG21	1:B:646:VAL:HG22	1.97	0.46
1:B:1037:LEU:HD21	1:B:1058:LYS:HG3	1.98	0.46
1:B:562:TYR:HB2	1:B:564:ILE:HG12	1.98	0.46
1:B:890:GLU:HG3	1:B:936:TYR:OH	2.15	0.46
1:B:753:ARG:NH1	1:B:781:GLY:HA2	2.30	0.46
1:B:1720:GLU:HB2	1:B:1721:PRO:HD2	1.98	0.46
1:B:1657:ALA:HB1	1:B:1693:ARG:HB3	1.98	0.46
1:B:1774:GLN:N	1:B:1774:GLN:OE1	2.49	0.46
1:B:678:ASN:HD22	1:B:681:ARG:HH21	1.64	0.45
1:B:1467:LEU:O	1:B:1470:ILE:HG13	2.16	0.45
1:B:1733:HIS:CD2	1:B:1733:HIS:N	2.84	0.45
1:B:1481:ILE:HG22	1:B:1483:ARG:HG2	1.97	0.45
1:B:1493:SER:HB3	1:B:1516:PRO:HD3	1.98	0.45
1:B:1452:VAL:HB	1:B:1488:VAL:HG13	1.98	0.45
1:B:777:LEU:HD22	1:B:782:PHE:HD2	1.82	0.45
1:B:2097:PRO:HG2	1:B:2102:HIS:CD2	2.52	0.45
1:B:815:LEU:HD12	1:B:819:VAL:HB	1.99	0.45
1:B:1184:LEU:HD12	1:B:1270:VAL:HG11	1.99	0.45
1:B:1923:ILE:HD11	1:B:1942:ALA:HB1	1.98	0.45
1:B:421:HIS:CE1	1:B:846:ALA:HB2	2.52	0.45
1:B:704:MET:HG2	1:B:870:ILE:HG21	1.98	0.44
1:B:819:VAL:O	1:B:855:ARG:NH2	2.41	0.44
1:B:1345:ASN:HA	1:B:1487:ILE:O	2.17	0.44
1:B:577:LYS:NZ	1:B:1537:THR:HG21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:920:LEU:HD23	1:B:920:LEU:HA	1.78	0.44
1:B:1180:LEU:HD23	1:B:1214:VAL:HG21	1.98	0.44
1:B:1554:SER:HB3	1:B:1659:HIS:ND1	2.32	0.44
1:B:442:TYR:CE1	1:B:707:ILE:HG12	2.52	0.44
1:B:409:LEU:H	1:B:959:THR:CG2	2.30	0.44
1:B:991:TYR:CE2	1:B:1097:GLU:HG3	2.48	0.44
1:B:1156:LEU:HD12	1:B:1156:LEU:HA	1.70	0.44
1:B:1733:HIS:HB2	1:B:1826:TYR:CE1	2.52	0.44
1:B:1829:ILE:HD13	1:B:1829:ILE:HA	1.75	0.44
1:B:475:PHE:CE2	1:B:511:ASN:HB3	2.53	0.44
1:B:554:SER:O	1:B:558:ARG:HG2	2.17	0.44
1:B:822:PRO:HB2	1:B:858:ARG:HA	1.99	0.44
1:B:2067:VAL:HB	1:B:2107:TYR:HB2	1.97	0.44
1:B:703:ILE:O	1:B:707:ILE:HG13	2.17	0.44
1:B:1122:MET:SD	1:B:1130:ARG:HB2	2.57	0.44
1:B:588:CYS:SG	1:B:593:TRP:HB2	2.58	0.44
1:B:1201:GLU:HG2	1:B:1253:THR:HG23	2.00	0.44
1:B:1294:LYS:HD3	1:B:1295:TYR:H	1.82	0.44
1:B:1052:ILE:HG13	1:B:1053:GLU:H	1.82	0.44
1:B:1262:LEU:HD23	1:B:1263:PRO:HD2	1.99	0.44
1:B:1577:LEU:HD13	1:B:1617:VAL:HG12	1.99	0.44
1:B:828:ILE:HD12	1:B:869:LEU:HD12	2.00	0.43
1:B:1268:ILE:HG13	1:B:1282:LEU:HB3	2.00	0.43
1:B:1963:LEU:HD13	1:B:2007:VAL:HG13	1.99	0.43
1:B:1380:THR:HG21	1:B:1385:LEU:HB2	1.99	0.43
1:B:1693:ARG:HB2	1:B:1695:LEU:HD12	1.99	0.43
1:B:409:LEU:HB2	1:B:959:THR:HG21	1.99	0.43
1:B:760:GLU:HG2	1:B:805:HIS:HA	2.00	0.43
1:B:1205:THR:HG23	1:B:1249:GLU:HG2	2.00	0.43
1:B:608:LEU:HD23	1:B:608:LEU:HA	1.85	0.43
1:B:819:VAL:HG12	1:B:821:LEU:HB2	1.99	0.43
1:B:1099:VAL:CG2	1:B:1104:TRP:HB2	2.48	0.43
1:B:1375:ARG:NH2	1:B:1419:LEU:O	2.52	0.43
1:B:1763:ARG:HA	1:B:1763:ARG:HD2	1.77	0.43
1:B:952:ARG:HD3	1:B:956:LEU:HD13	2.00	0.43
1:B:448:PRO:HA	1:B:686:GLU:HG3	1.99	0.43
1:B:559:LEU:HD13	1:B:564:ILE:HB	1.99	0.43
1:B:1006:LYS:HD3	1:B:1006:LYS:HA	1.83	0.43
1:B:1026:ASN:OD1	1:B:1026:ASN:N	2.52	0.43
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	2.00	0.43
1:B:1364:ILE:HA	1:B:1367:MET:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:PRO:HG3	1:B:1104:TRP:CE2	2.53	0.43
1:B:1290:ILE:HG13	1:B:1290:ILE:H	1.71	0.43
1:B:1367:MET:HE1	1:B:1375:ARG:N	2.33	0.43
1:B:1600:TYR:O	1:B:1603:LYS:HG2	2.18	0.43
1:B:1577:LEU:HD11	1:B:1615:ASN:CB	2.46	0.43
1:B:1683:ASP:O	1:B:1687:MET:HG3	2.19	0.43
1:B:513:ALA:HB2	1:B:651:LEU:HD11	2.01	0.43
1:B:1469:VAL:HG21	1:B:1735:HIS:CD2	2.54	0.43
1:B:1755:LEU:O	1:B:1761:TYR:HB2	2.19	0.43
1:B:726:HIS:HB3	1:B:833:VAL:HG23	2.01	0.42
1:B:1394:TYR:CD1	1:B:1398:GLN:HB3	2.53	0.42
1:B:1648:ARG:HD3	1:B:1679:TYR:CZ	2.54	0.42
1:B:1750:ASP:HA	1:B:1753:ASP:HB2	2.00	0.42
1:B:616:GLU:HA	1:B:618:HIS:CE1	2.54	0.42
1:B:1457:HIS:HB3	1:B:1494:LEU:HD11	2.01	0.42
1:B:1662:ILE:HG12	1:B:1703:VAL:HG22	2.01	0.42
1:B:1594:GLU:O	1:B:1598:ILE:HG13	2.19	0.42
1:B:1733:HIS:HD1	1:B:1826:TYR:HH	1.66	0.42
1:B:619:LEU:HD23	1:B:628:LEU:HG	2.02	0.42
1:B:1012:ILE:H	1:B:1012:ILE:HD12	1.83	0.42
1:B:1332:GLN:NE2	1:B:1358:ILE:HD11	2.33	0.42
1:B:1459:ILE:H	1:B:1459:ILE:HG12	1.63	0.42
1:B:624:ARG:O	1:B:627:VAL:HG22	2.20	0.42
1:B:731:THR:HG21	1:B:786:HIS:HD2	1.84	0.42
1:B:785:HIS:CE1	1:B:815:LEU:HD13	2.55	0.42
1:B:1556:LYS:HE2	1:B:1556:LYS:HB3	1.72	0.42
1:B:1187:SER:OG	1:B:1203:THR:HB	2.19	0.42
1:B:1558:PRO:HA	1:B:1642:GLN:O	2.20	0.42
1:B:1805:GLU:HG3	1:B:1806:ASP:OD1	2.20	0.42
1:B:1849:ILE:HD13	1:B:1849:ILE:HA	1.95	0.42
1:B:577:LYS:O	1:B:580:ILE:HG22	2.19	0.42
1:B:628:LEU:HD23	1:B:628:LEU:HA	1.84	0.42
1:B:722:LEU:HA	1:B:722:LEU:HD12	1.85	0.42
1:B:962:LEU:HD23	1:B:962:LEU:HA	1.93	0.42
1:B:1530:PHE:O	1:B:1532:ILE:N	2.51	0.42
1:B:618:HIS:CE1	1:B:653:ALA:H	2.38	0.42
1:B:1435:LEU:O	1:B:1442:ARG:NH1	2.53	0.42
1:B:1566:ARG:CB	1:B:1621:HIS:HB2	2.50	0.42
1:B:1899:LEU:HD23	1:B:1899:LEU:HA	1.93	0.42
1:B:1043:ARG:NH2	1:B:1070:LEU:HD22	2.35	0.42
1:B:1400:ARG:HA	1:B:1400:ARG:HD3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:ILE:HD11	1:B:650:GLY:HA2	2.02	0.41
1:B:739:ARG:NH2	1:B:777:LEU:HD23	2.35	0.41
1:B:1117:MET:HG2	1:B:1276:LEU:HD11	2.02	0.41
1:B:1123:TRP:HD1	1:B:1126:MET:HE1	1.85	0.41
1:B:1493:SER:CB	1:B:1516:PRO:HD3	2.50	0.41
1:B:654:THR:HG21	1:B:677:ASP:HA	2.02	0.41
1:B:760:GLU:O	1:B:764:THR:HG23	2.19	0.41
1:B:1613:LEU:HD23	1:B:1613:LEU:HA	1.87	0.41
1:B:1666:THR:HA	1:B:1679:TYR:CE2	2.55	0.41
1:B:1881:ASN:N	1:B:1882:PRO:HD3	2.34	0.41
1:B:1609:LEU:HA	1:B:1612:THR:HG22	2.02	0.41
1:B:1855:TYR:CZ	1:B:1915:ILE:HG23	2.56	0.41
1:B:1023:GLU:OE1	1:B:1023:GLU:N	2.50	0.41
1:B:1035:LEU:HG	1:B:1039:LYS:HE2	2.01	0.41
1:B:1335:VAL:HG22	1:B:1339:VAL:HG23	2.02	0.41
1:B:1358:ILE:O	1:B:1361:GLU:HB2	2.21	0.41
1:B:1768:PRO:HB3	1:B:1773:LEU:HG	2.03	0.41
1:B:594:ASP:O	1:B:598:ARG:HG2	2.20	0.41
1:B:542:ALA:O	1:B:590:PRO:HD3	2.21	0.41
1:B:2000:THR:HG23	1:B:2003:GLN:H	1.86	0.41
1:B:1714:PHE:O	1:B:1715:LYS:C	2.59	0.41
1:B:1781:LEU:O	1:B:1785:LEU:HG	2.20	0.41
1:B:603:ARG:HE	1:B:607:GLN:HG3	1.86	0.41
1:B:1139:VAL:HG22	1:B:1167:MET:SD	2.61	0.41
1:B:1346:VAL:O	1:B:1488:VAL:HA	2.21	0.41
1:B:1397:PHE:HD1	1:B:1401:LEU:HD12	1.85	0.41
1:B:1566:ARG:HG3	1:B:1567:LYS:N	2.34	0.41
1:B:1822:TYR:O	1:B:1921:ARG:HD3	2.21	0.41
1:B:1879:LEU:HD23	1:B:1880:ASN:O	2.21	0.41
1:B:416:PHE:HB3	1:B:422:PHE:HB2	2.03	0.41
1:B:840:ARG:NH1	1:B:842:THR:HG22	2.36	0.41
1:B:1342:SER:C	1:B:1366:ARG:HH22	2.24	0.41
1:B:1945:LEU:O	1:B:1949:VAL:HG13	2.21	0.41
1:B:721:VAL:HA	1:B:825:THR:HB	2.02	0.40
1:B:1237:GLU:HG2	1:B:1709:SER:HB2	2.02	0.40
1:B:1542:MET:O	1:B:1546:VAL:HG13	2.21	0.40
1:B:1577:LEU:HA	1:B:1577:LEU:HD12	1.73	0.40
1:B:1800:LYS:O	1:B:1813:LEU:HD12	2.20	0.40
1:B:1887:PRO:O	1:B:1891:THR:HG23	2.21	0.40
1:B:853:LEU:HA	1:B:853:LEU:HD23	1.84	0.40
1:B:1901:ARG:HH21	1:B:2055:LEU:HD11	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1616:GLY:O	1:B:1641:ILE:HG23	2.21	0.40
1:B:1654:MET:HE2	1:B:1654:MET:HB3	1.87	0.40
1:B:1841:LYS:O	1:B:1845:LEU:HD13	2.21	0.40
1:B:603:ARG:O	1:B:607:GLN:HB2	2.22	0.40
1:B:615:ASP:HA	1:B:651:LEU:HB2	2.02	0.40
1:B:1548:HIS:HB3	1:B:1552:LYS:HZ2	1.87	0.40
1:B:1566:ARG:O	1:B:1569:THR:OG1	2.21	0.40
1:B:1607:SER:O	1:B:1611:GLU:HG2	2.21	0.40
1:B:1813:LEU:HD13	1:B:1814:ASN:N	2.36	0.40
1:B:1968:SER:HA	1:B:1971:ILE:HG12	2.04	0.40
1:B:1561:VAL:O	1:B:1645:VAL:HA	2.21	0.40
1:B:1672:LYS:HD2	1:B:1887:PRO:HG3	2.04	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	B	1722/1747 (99%)	1625 (94%)	96 (6%)	1 (0%)	51 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1713	PHE

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	1542/1560 (99%)	1482 (96%)	60 (4%)	32 64

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	430	LEU
1	B	439	ARG
1	B	447	VAL
1	B	462	LEU
1	B	489	TYR
1	B	526	ASN
1	B	561	THR
1	B	606	THR
1	B	618	HIS
1	B	621	HIS
1	B	638	ASN
1	B	654	THR
1	B	770	LYS
1	B	771	ASN
1	B	793	ASP
1	B	844	LEU
1	B	878	TYR
1	B	928	ARG
1	B	993	ILE
1	B	995	ASN
1	B	1037	LEU
1	B	1040	LEU
1	B	1191	GLN
1	B	1218	SER
1	B	1262	LEU
1	B	1269	ARG
1	B	1331	ILE
1	B	1335	VAL
1	B	1368	LEU
1	B	1375	ARG
1	B	1380	THR
1	B	1394	TYR
1	B	1406	VAL
1	B	1475	ARG
1	B	1487	ILE
1	B	1488	VAL

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Mol	Chain	Res	Type
1	B	1490	LEU
1	B	1499	ASP
1	B	1517	ASN
1	B	1555	PRO
1	B	1566	ARG
1	B	1580	CYS
1	B	1583	ASP
1	B	1607	SER
1	B	1617	VAL
1	B	1678	ASP
1	B	1697	ASP
1	B	1745	ILE
1	B	1809	ASP
1	B	1813	LEU
1	B	1841	LYS
1	B	1863	HIS
1	B	1904	LEU
1	B	1930	LEU
1	B	1963	LEU
1	B	1966	PHE
1	B	2025	ASP
1	B	2056	PHE
1	B	2068	ILE
1	B	2102	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

1 ligand is 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	QA9	B	2201	-	13,14,14	1.78	4 (30%)	17,20,20	4.43	4 (23%)

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	QA9	B	2201	-	-	4/9/11/11	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2201	QA9	S05-N04	3.24	1.71	1.64
2	B	2201	QA9	C02-N01	2.79	1.46	1.34
2	B	2201	QA9	O07-S05	2.58	1.46	1.43
2	B	2201	QA9	C08-S05	2.51	1.80	1.76

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2201	QA9	O07-S05-O06	-16.67	99.06	119.55
2	B	2201	QA9	C08-S05-N04	4.82	113.28	105.97
2	B	2201	QA9	O07-S05-N04	3.53	116.67	106.74
2	B	2201	QA9	O06-S05-C08	2.96	111.62	107.97

There are no chirality outliers.

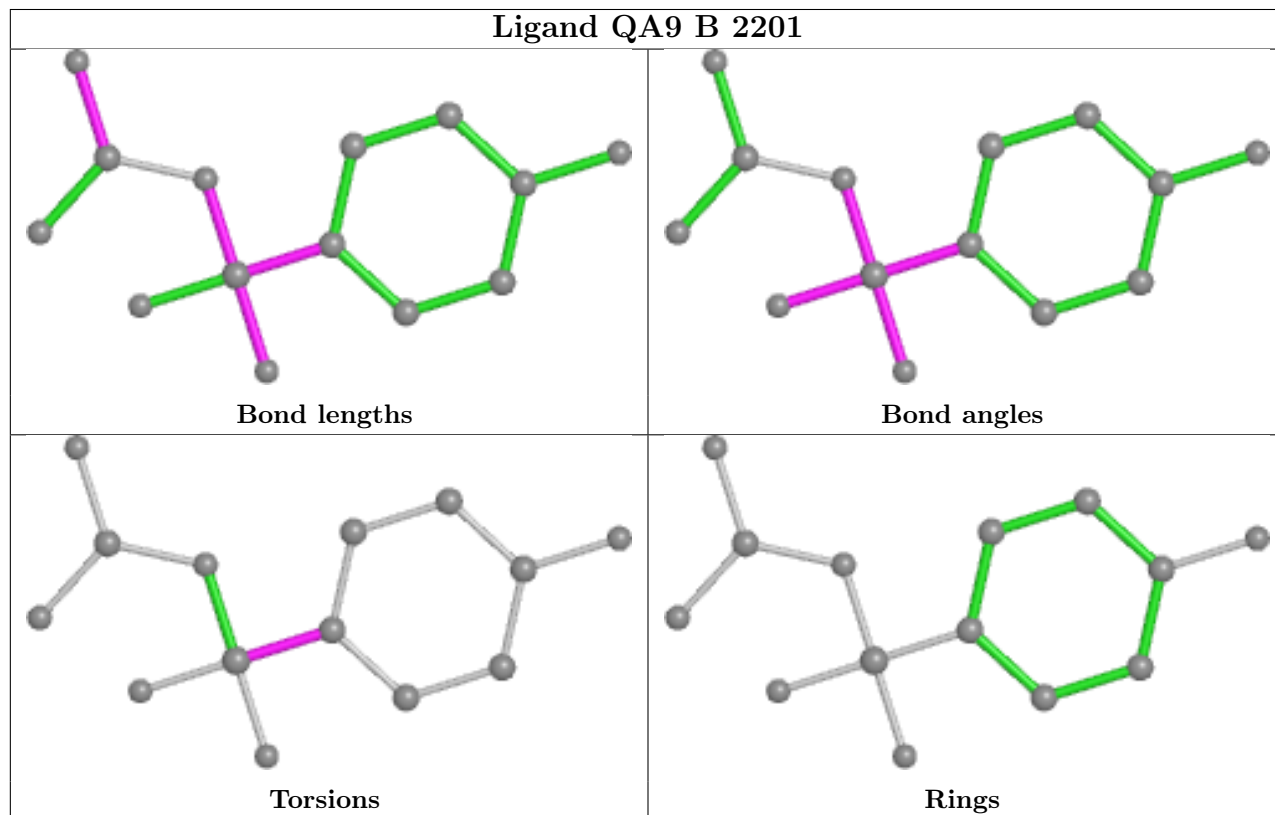
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2201	QA9	C14-C08-S05-O06
2	B	2201	QA9	C09-C08-S05-O06
2	B	2201	QA9	C14-C08-S05-N04
2	B	2201	QA9	C09-C08-S05-N04

There are no ring outliers.

No monomer is involved in short contacts.

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	B	1724/1747 (98%)	0.75	236 (13%) 3 2	52, 112, 198, 330	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1985	ILE	10.4
1	B	572	ASP	9.2
1	B	1988	MET	8.5
1	B	571	GLY	8.1
1	B	783	ALA	7.9
1	B	757	ALA	7.7
1	B	573	HIS	7.4
1	B	2010	PHE	7.3
1	B	1587	GLN	7.1
1	B	2124	VAL	7.0
1	B	2015	PRO	6.6
1	B	1979	VAL	6.2
1	B	774	LEU	6.2
1	B	442	TYR	6.0
1	B	763	ARG	5.9
1	B	694	GLU	5.7
1	B	1997	LEU	5.7
1	B	692	ILE	5.6
1	B	1963	LEU	5.5
1	B	1481	ILE	5.4
1	B	829	LYS	5.3
1	B	756	SER	5.3
1	B	780	TYR	5.2
1	B	2014	TYR	5.2
1	B	1993	ARG	5.2
1	B	530	THR	5.2
1	B	784	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	435	PHE	5.2
1	B	782	PHE	5.2
1	B	2007	VAL	5.0
1	B	754	GLU	5.0
1	B	2120	TYR	5.0
1	B	1964	PRO	5.0
1	B	1761	TYR	5.0
1	B	527	MET	4.7
1	B	575	LEU	4.7
1	B	2019	LEU	4.7
1	B	778	LEU	4.6
1	B	753	ARG	4.6
1	B	1321	TYR	4.6
1	B	467	LEU	4.5
1	B	2016	ASN	4.5
1	B	2052	ILE	4.4
1	B	1975	THR	4.3
1	B	2123	SER	4.3
1	B	1960	LEU	4.2
1	B	2041	LEU	4.2
1	B	2006	ASP	4.1
1	B	876	LEU	4.1
1	B	2101	ALA	4.0
1	B	1148	PHE	4.0
1	B	1165	ILE	3.9
1	B	2005	ALA	3.9
1	B	1775	GLY	3.8
1	B	1037	LEU	3.8
1	B	877	GLN	3.8
1	B	690	VAL	3.7
1	B	2106	LEU	3.7
1	B	1050	GLU	3.7
1	B	2092	LEU	3.6
1	B	422	PHE	3.6
1	B	1317	PHE	3.6
1	B	1773	LEU	3.6
1	B	2084	LEU	3.6
1	B	2042	GLU	3.5
1	B	743	LEU	3.5
1	B	736	ARG	3.5
1	B	2008	ALA	3.5
1	B	2004	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	712	ILE	3.4
1	B	588	CYS	3.3
1	B	2102	HIS	3.3
1	B	445	VAL	3.3
1	B	1336	PHE	3.3
1	B	1965	HIS	3.3
1	B	713	MET	3.3
1	B	879	TYR	3.2
1	B	1802	ILE	3.2
1	B	1135	LEU	3.2
1	B	1241	LEU	3.2
1	B	1776	ILE	3.2
1	B	1996	LEU	3.2
1	B	974	LYS	3.1
1	B	2059	LYS	3.1
1	B	545	ARG	3.1
1	B	1480	GLN	3.1
1	B	2017	ILE	3.1
1	B	589	THR	3.1
1	B	1423	ASN	3.1
1	B	1682	TYR	3.1
1	B	1986	MET	3.0
1	B	1732	MET	3.0
1	B	440	LYS	3.0
1	B	1977	LYS	3.0
1	B	1974	CYS	3.0
1	B	444	GLU	3.0
1	B	576	CYS	3.0
1	B	1443	LYS	2.9
1	B	1752	VAL	2.9
1	B	1132	PHE	2.9
1	B	1871	LEU	2.9
1	B	2061	GLU	2.9
1	B	1365	LEU	2.9
1	B	1601	LEU	2.9
1	B	464	VAL	2.8
1	B	506	GLY	2.8
1	B	437	ARG	2.8
1	B	2082	LEU	2.8
1	B	466	LYS	2.8
1	B	723	VAL	2.8
1	B	570	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	709	TYR	2.8
1	B	1051	SER	2.8
1	B	861	TYR	2.8
1	B	1961	LYS	2.7
1	B	1342	SER	2.7
1	B	724	PHE	2.7
1	B	1987	GLU	2.7
1	B	574	GLN	2.7
1	B	1577	LEU	2.7
1	B	1796	LEU	2.7
1	B	562	TYR	2.7
1	B	591	GLU	2.7
1	B	402	ALA	2.7
1	B	508	GLY	2.7
1	B	822	PRO	2.7
1	B	720	GLN	2.7
1	B	1846	ILE	2.7
1	B	1604	LEU	2.7
1	B	1962	GLN	2.6
1	B	2035	VAL	2.6
1	B	715	HIS	2.6
1	B	1463	ASN	2.6
1	B	2091	LYS	2.6
1	B	475	PHE	2.6
1	B	2038	LEU	2.6
1	B	446	HIS	2.6
1	B	853	LEU	2.6
1	B	693	THR	2.6
1	B	682	PRO	2.6
1	B	528	ASP	2.5
1	B	869	LEU	2.5
1	B	546	SER	2.5
1	B	1312	LEU	2.5
1	B	471	ALA	2.5
1	B	569	LEU	2.5
1	B	961	ALA	2.5
1	B	493	LEU	2.5
1	B	2043	ARG	2.5
1	B	1368	LEU	2.5
1	B	820	ASN	2.5
1	B	2087	LYS	2.5
1	B	1984	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1788	LEU	2.5
1	B	1586	ARG	2.4
1	B	979	PHE	2.4
1	B	1417	LYS	2.4
1	B	1177	TYR	2.4
1	B	433	GLY	2.4
1	B	460	GLN	2.4
1	B	2040	GLN	2.4
1	B	526	ASN	2.4
1	B	1620	LEU	2.4
1	B	1784	HIS	2.4
1	B	1150	PHE	2.4
1	B	590	PRO	2.4
1	B	863	THR	2.4
1	B	1461	GLY	2.4
1	B	544	MET	2.4
1	B	719	ASN	2.4
1	B	1597	LEU	2.4
1	B	2034	PRO	2.3
1	B	1764	MET	2.3
1	B	770	LYS	2.3
1	B	518	LEU	2.3
1	B	1331	ILE	2.3
1	B	729	LYS	2.3
1	B	2049	GLY	2.3
1	B	972	TYR	2.3
1	B	1793	LEU	2.3
1	B	748	LEU	2.3
1	B	1995	ALA	2.3
1	B	701	PHE	2.3
1	B	758	SER	2.3
1	B	427	ARG	2.3
1	B	1971	ILE	2.3
1	B	1878	LYS	2.3
1	B	411	LEU	2.2
1	B	1494	LEU	2.2
1	B	938	ILE	2.2
1	B	2046	GLU	2.2
1	B	819	VAL	2.2
1	B	734	THR	2.2
1	B	469	LYS	2.2
1	B	592	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1286	PHE	2.2
1	B	855	ARG	2.2
1	B	2116	CYS	2.2
1	B	711	LYS	2.2
1	B	716	ALA	2.2
1	B	2114	MET	2.2
1	B	488	LEU	2.2
1	B	750	LEU	2.2
1	B	802	ALA	2.2
1	B	1246	ALA	2.2
1	B	2079	ILE	2.2
1	B	1410	GLY	2.1
1	B	501	LEU	2.1
1	B	984	LEU	2.1
1	B	1901	ARG	2.1
1	B	717	GLY	2.1
1	B	2024	VAL	2.1
1	B	1035	LEU	2.1
1	B	1137	GLU	2.1
1	B	1954	TRP	2.1
1	B	510	THR	2.1
1	B	959	THR	2.1
1	B	414	LEU	2.1
1	B	821	LEU	2.1
1	B	2023	VAL	2.1
1	B	1883	LYS	2.1
1	B	2083	THR	2.1
1	B	2011	CYS	2.1
1	B	438	GLN	2.0
1	B	1004	LEU	2.0
1	B	1322	GLN	2.0
1	B	593	TRP	2.0
1	B	1978	GLY	2.0
1	B	2022	GLU	2.0
1	B	852	MET	2.0
1	B	705	ASN	2.0
1	B	621	HIS	2.0
1	B	568	GLU	2.0
1	B	854	GLY	2.0
1	B	1151	GLU	2.0
1	B	2100	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](#)

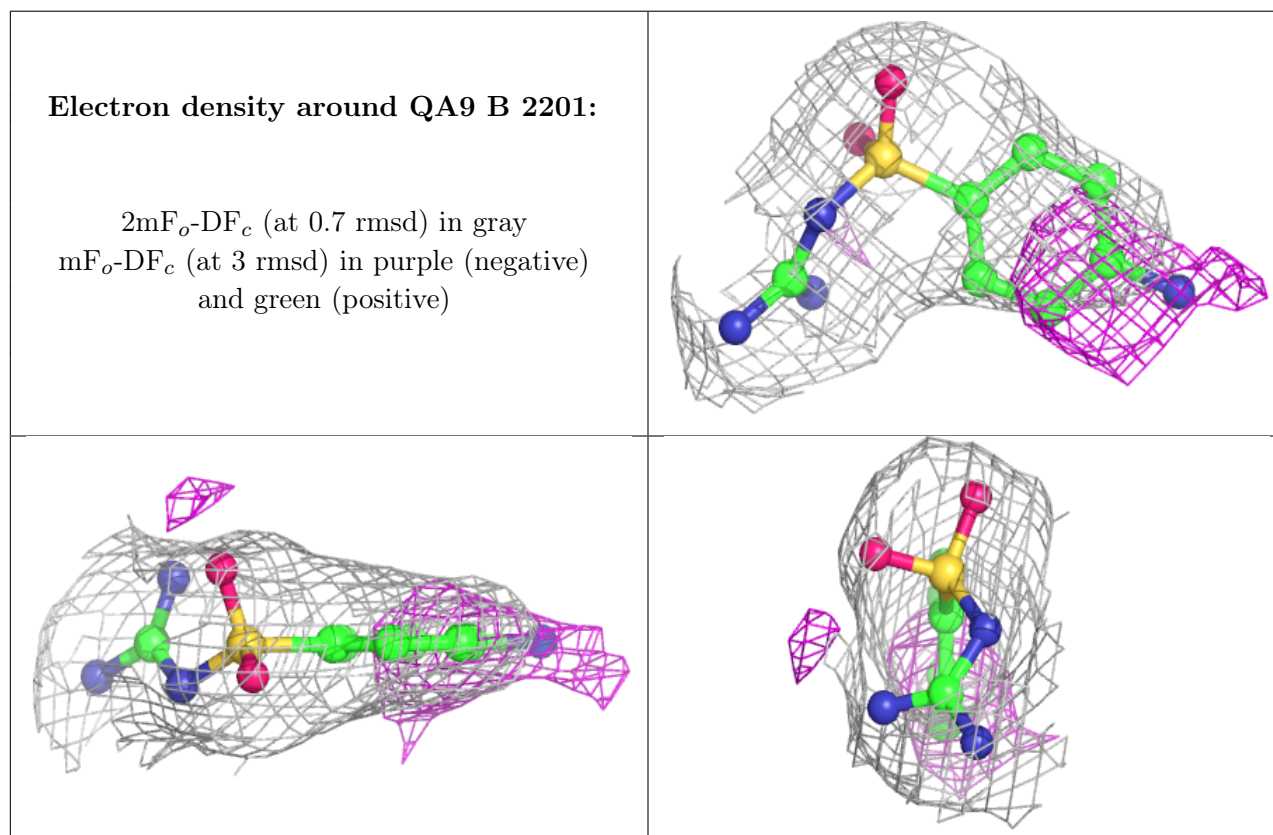
There are no monosaccharides in this entry.

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	QA9	B	2201	14/14	0.91	0.25	50,57,66,94	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.