



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 11:29 PM UTC

PDB ID : 8BCH / pdb\_00008bch  
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](mailto: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>.

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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

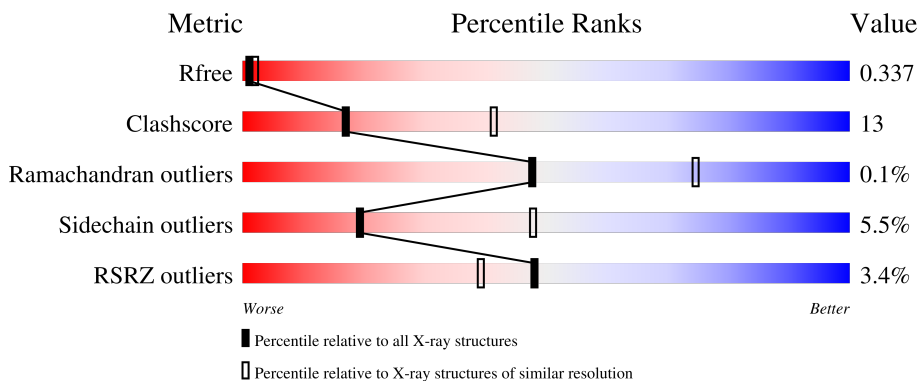
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.87 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))
$R_{free}$	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (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  $\geq 3$ , 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.

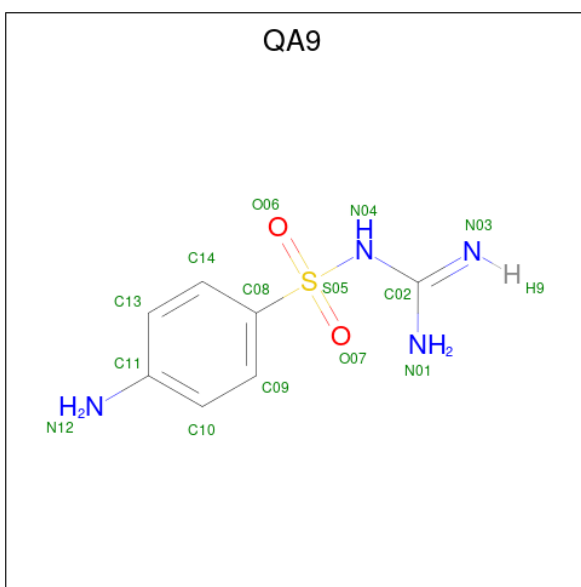
- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

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 (CCD ID: QA9) (formula: C<sub>7</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).

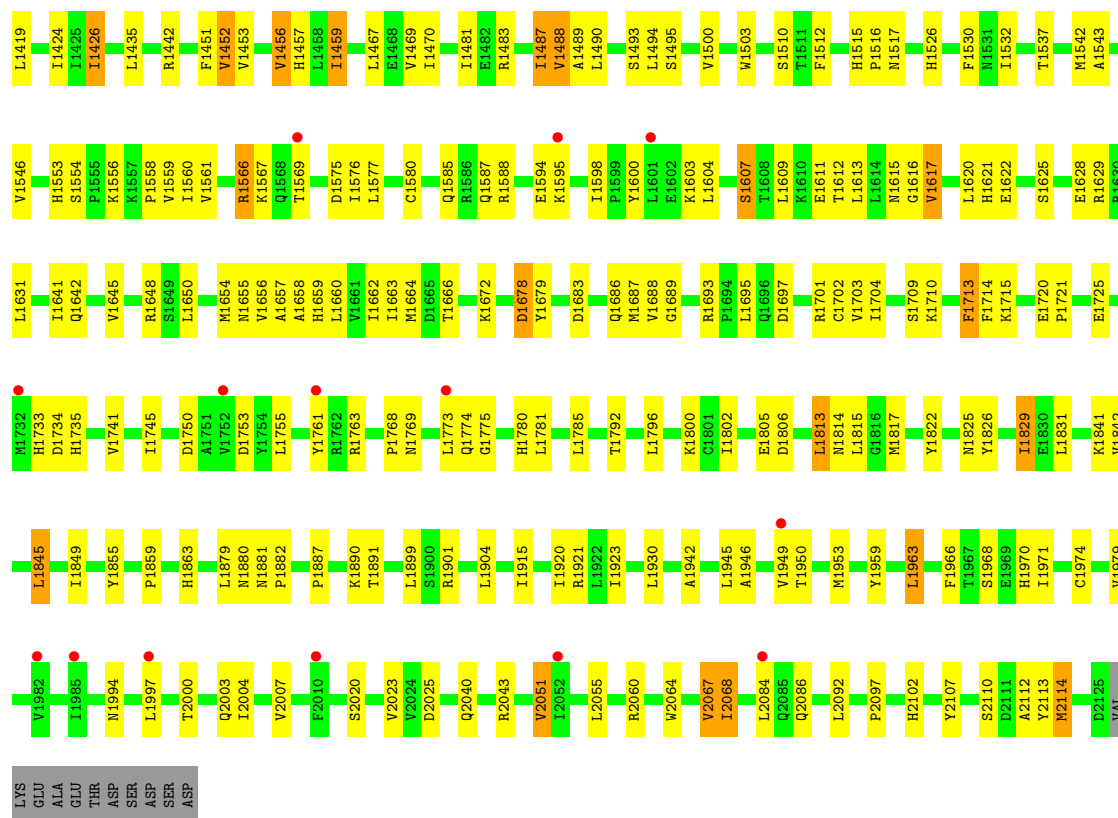


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	14	7	4	2	1	0	0

- Molecule 3 is water.

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





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 93.4 (47.20-2.87)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 2.86Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, $R_{free}$	0.281 , 0.337 0.281 , 0.337	Depositor DCC
$R_{free}$ test set	2013 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.8	Xtrriage
Anisotropy	0.412	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 98.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
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	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.15	0/14153	0.35	1/19177 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	441	GLY	CA-C-O	-5.77	116.58	122.59

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	354	0
2	B	14	0	0	0	0
3	B	11	0	0	0	0
All	All	13884	0	14001	354	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 13.

All (354) 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
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:1075:PHE:HA	1:B:1078:MET:HE3	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ILE:HG22	1:B:586:ILE:HB	1.81	0.62
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:1859:PRO:O	1:B:1890:LYS:NZ	2.31	0.62
1:B:929:MET:HE2	1:B:949:LEU:HD13	1.80	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: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:704:MET:HE2	1:B:829:LYS:HE3	1.89	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1741:VAL:HG13	1:B:1817:MET:HE2	1.88	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
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.88	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:929:MET:HE3	1:B:938:ILE:HD11	1.91	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:512:VAL:HA	1:B:515:MET:HE2	1.92	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:1566:ARG:O	1:B:1569:THR:OG1	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:539:ILE:HD11	1:B:612:ILE:HG12	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:550:GLU:HG3	1:B:551:MET:HE2	1.94	0.50
1:B:627:VAL:HG12	1:B:900:MET:HE1	1.93	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:1114:LEU:HA	1:B:1117:MET:HE3	1.95	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:517:MET:HE3	1:B:613:ILE:HD12	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1367:MET:HE1	1:B:1375:ARG:N	2.30	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:1146:LYS:NZ	1:B:1164:LEU:O	2.44	0.46
1:B:1657:ALA:HB1	1:B:1693:ARG:HB3	1.98	0.46
1:B:1714:PHE:O	1:B:1715:LYS:C	2.59	0.46
1:B:1774:GLN:N	1:B:1774:GLN:OE1	2.49	0.46
1:B:419:GLY:C	1:B:421:HIS:H	2.23	0.45
1:B:678:ASN:HD22	1:B:681:ARG:HH21	1.64	0.45
1:B:1342:SER:C	1:B:1366:ARG:HH22	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1678:ASP:OD1	1:B:1710:LYS:NZ	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1600:TYR:O	1:B:1603:LYS:HG2	2.18	0.43
1:B:457:SER:C	1:B:459:GLU:H	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1713:PHE:O	1:B:1714:PHE:C	2.62	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
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: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:1650:LEU:HB3	1:B:1654:MET:HE3	2.02	0.41
1:B:1953:MET:HE1	1:B:1959:TYR:HA	2.02	0.41
1:B:2000:THR:HG23	1:B:2003:GLN:H	1.86	0.41
1:B:1226:GLU:CD	1:B:1269:ARG:HH11	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1945:LEU:O	1:B:1949:VAL:HG13	2.21	0.41
1:B:1953:MET:HE2	1:B:2114:MET:HE2	2.02	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
1:B:1616:GLY:O	1:B:1641:ILE:HG23	2.21	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:632:VAL:O	1:B:633:ALA:C	2.65	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:656:PRO:HD3	1:B:885:GLN:C	2.47	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%)	48   74

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%)	1457 (94%)	85 (6%)	19 48

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	423	MET
1	B	429	GLN
1	B	439	ARG
1	B	447	VAL
1	B	462	LEU
1	B	489	TYR
1	B	512	VAL
1	B	526	ASN
1	B	531	ILE
1	B	561	THR
1	B	564	ILE
1	B	580	ILE
1	B	606	THR
1	B	610	ARG
1	B	617	ILE
1	B	618	HIS
1	B	638	ASN
1	B	643	GLN
1	B	646	VAL
1	B	654	THR
1	B	667	VAL
1	B	685	LEU
1	B	690	VAL
1	B	722	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	770	LYS
1	B	771	ASN
1	B	775	LYS
1	B	829	LYS
1	B	844	LEU
1	B	878	TYR
1	B	894	VAL
1	B	928	ARG
1	B	956	LEU
1	B	993	ILE
1	B	1037	LEU
1	B	1040	LEU
1	B	1052	ILE
1	B	1071	LYS
1	B	1082	VAL
1	B	1135	LEU
1	B	1191	GLN
1	B	1202	LEU
1	B	1218	SER
1	B	1262	LEU
1	B	1271	VAL
1	B	1331	ILE
1	B	1335	VAL
1	B	1352	THR
1	B	1358	ILE
1	B	1368	LEU
1	B	1375	ARG
1	B	1380	THR
1	B	1406	VAL
1	B	1426	ILE
1	B	1452	VAL
1	B	1456	VAL
1	B	1459	ILE
1	B	1487	ILE
1	B	1488	VAL
1	B	1490	LEU
1	B	1517	ASN
1	B	1559	VAL
1	B	1566	ARG
1	B	1580	CYS
1	B	1607	SER
1	B	1617	VAL

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Mol	Chain	Res	Type
1	B	1622	GLU
1	B	1655	ASN
1	B	1678	ASP
1	B	1697	ASP
1	B	1745	ILE
1	B	1813	LEU
1	B	1829	ILE
1	B	1831	LEU
1	B	1845	LEU
1	B	1863	HIS
1	B	1904	LEU
1	B	1930	LEU
1	B	1963	LEU
1	B	2023	VAL
1	B	2025	ASP
1	B	2051	VAL
1	B	2067	VAL
1	B	2068	ILE
1	B	2114	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	524	HIS
1	B	643	GLN
1	B	885	GLN
1	B	951	GLN
1	B	978	ASN
1	B	999	GLN
1	B	1179	HIS
1	B	1615	ASN
1	B	1898	HIS
1	B	2074	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	-	14,14,14	2.11	5 (35%)	17,20,20	4.45	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2201	QA9	C02-N04	4.42	1.46	1.36
2	B	2201	QA9	C02-N01	3.26	1.46	1.34
2	B	2201	QA9	S05-N04	2.93	1.71	1.64
2	B	2201	QA9	C08-S05	2.51	1.80	1.76
2	B	2201	QA9	O07-S05	2.51	1.46	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2201	QA9	O07-S05-O06	-16.85	99.06	119.52
2	B	2201	QA9	C08-S05-N04	4.52	113.28	106.06
2	B	2201	QA9	O07-S05-N04	3.46	116.67	106.77
2	B	2201	QA9	O06-S05-C08	2.89	111.62	107.98

There are no chirality outliers.

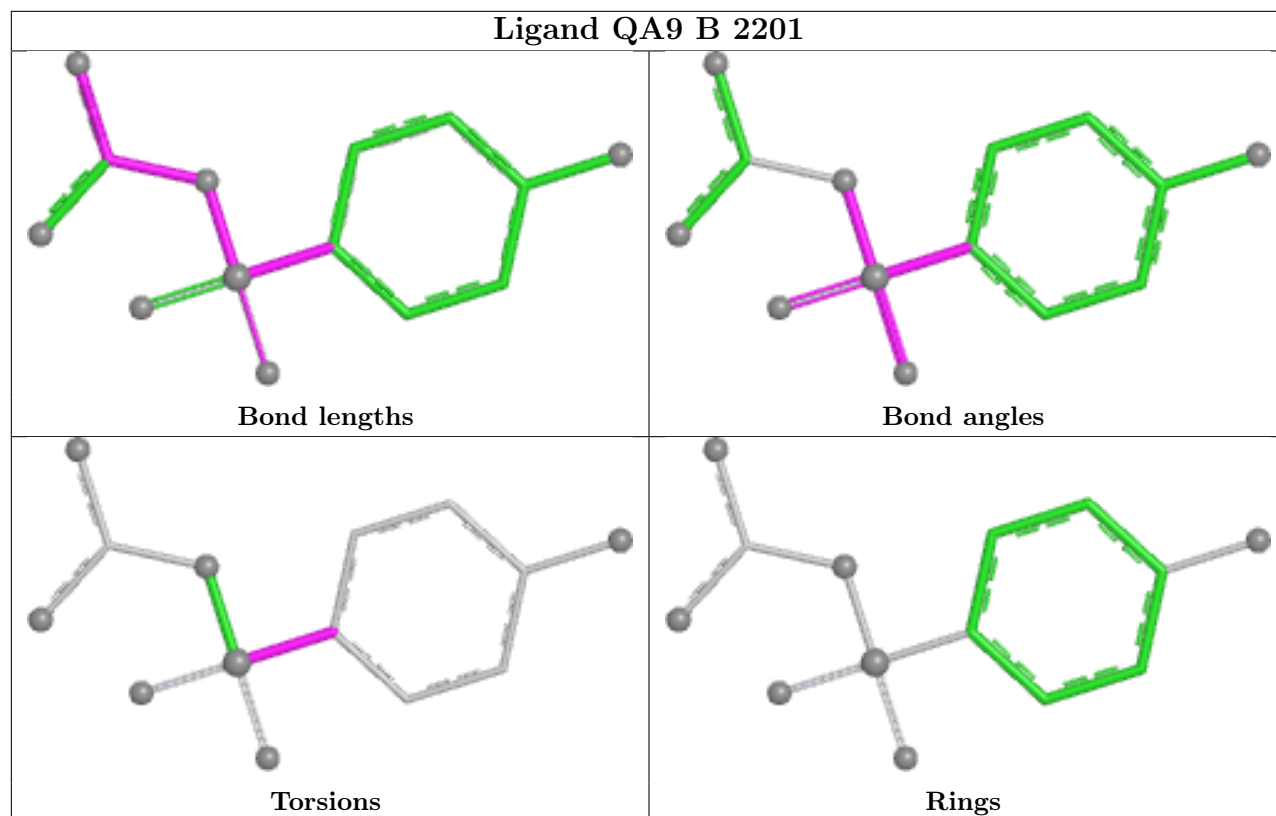
All (4) torsion outliers are listed below:

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	1724/1747 (98%)	0.49	58 (3%) 48 39	52, 112, 198, 330	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1985	ILE	4.6
1	B	1761	TYR	3.8
1	B	829	LYS	3.7
1	B	782	PHE	3.5
1	B	853	LEU	3.2
1	B	1139	VAL	3.0
1	B	1321	TYR	3.0
1	B	735	ALA	3.0
1	B	1051	SER	2.9
1	B	712	ILE	2.8
1	B	2052	ILE	2.8
1	B	1317	PHE	2.8
1	B	784	ILE	2.7
1	B	797	VAL	2.7
1	B	1246	ALA	2.6
1	B	1342	SER	2.6
1	B	861	TYR	2.5
1	B	802	ALA	2.5
1	B	2084	LEU	2.4
1	B	1595	LYS	2.4
1	B	1732	MET	2.4
1	B	783	ALA	2.4
1	B	894	VAL	2.4
1	B	2010	PHE	2.4
1	B	859	PRO	2.4
1	B	708	VAL	2.3
1	B	772	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1263	PRO	2.3
1	B	697	ALA	2.3
1	B	569	LEU	2.3
1	B	575	LEU	2.3
1	B	1773	LEU	2.2
1	B	1982	VAL	2.2
1	B	442	TYR	2.2
1	B	1148	PHE	2.2
1	B	1076	ALA	2.2
1	B	1949	VAL	2.2
1	B	570	THR	2.2
1	B	713	MET	2.2
1	B	876	LEU	2.2
1	B	1354	SER	2.2
1	B	1752	VAL	2.1
1	B	1569	THR	2.1
1	B	1234	LEU	2.1
1	B	846	ALA	2.1
1	B	723	VAL	2.1
1	B	863	THR	2.1
1	B	828	ILE	2.1
1	B	403	LEU	2.1
1	B	1997	LEU	2.1
1	B	507	ALA	2.1
1	B	1337	ASN	2.0
1	B	1601	LEU	2.0
1	B	508	GLY	2.0
1	B	821	LEU	2.0
1	B	1289	LEU	2.0
1	B	934	THR	2.0
1	B	780	TYR	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](#)

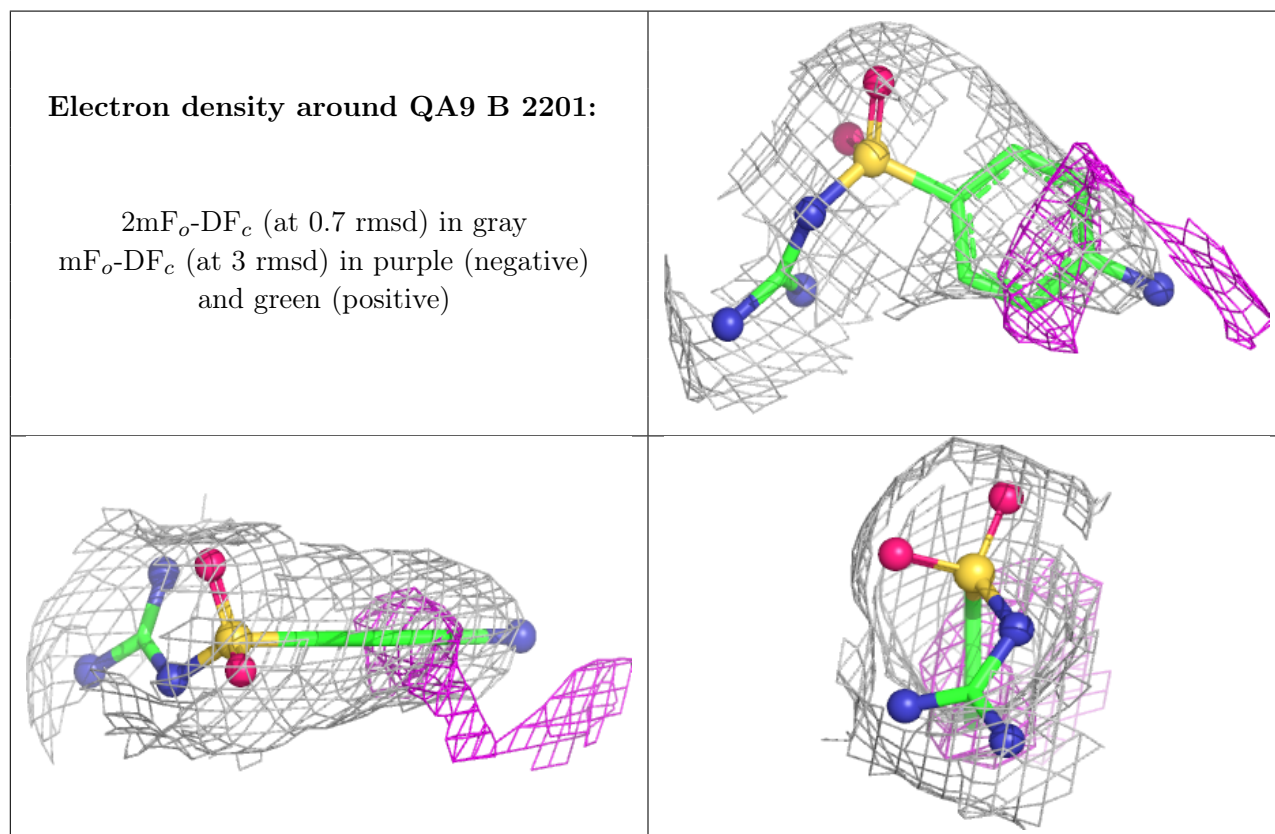
There are no oligosaccharides in this entry.

## 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	QA9	B	2201	14/14	0.88	0.11	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.