



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 07:01 PM EDT

PDB ID : 5URJ  
Title : Crystal structure of human BRR2 in complex with T-3905516  
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Deposited on : 2017-02-10  
Resolution : 2.75 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 : 4.02b-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

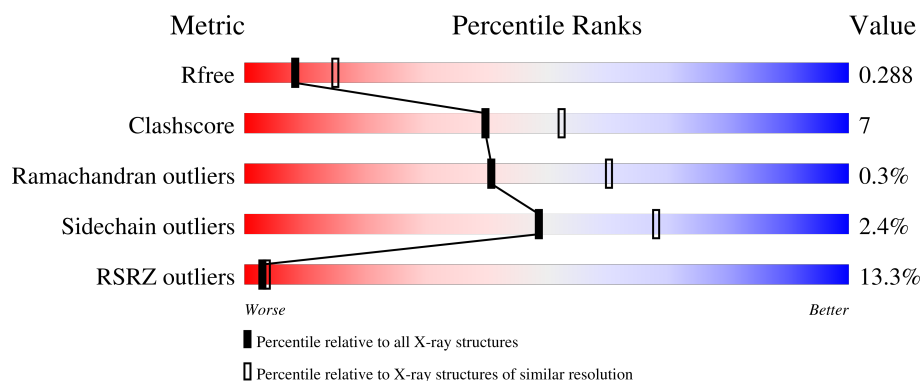
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	A	1738	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13745 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	A	1707	13688	8752	2339	2528	69	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

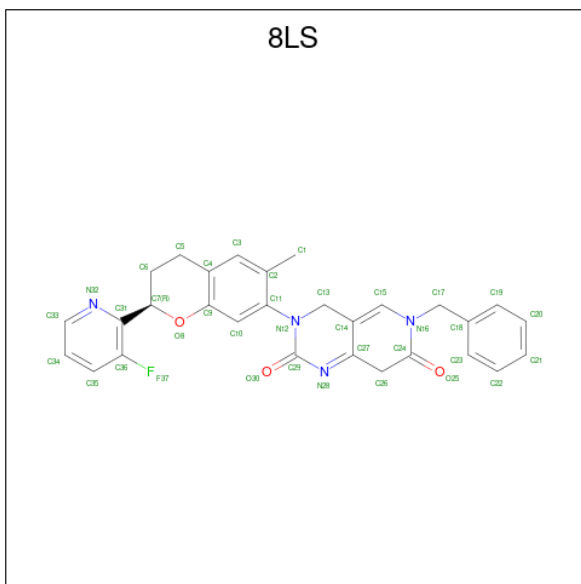
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	GLY	-	expression tag	UNP O75643
A	393	GLY	-	expression tag	UNP O75643
A	394	SER	-	expression tag	UNP O75643

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0

- Molecule 3 is 6-benzyl-3-[(2R)-2-(3-fluoropyridin-2-yl)-6-methyl-3,4-dihydro-2H-1-benzopyran-7-yl]-4,6-dihydropyrido[4,3-d]pyrimidine-2,7(3H,8H)-dione (three-letter code: 8LS) (formula: C<sub>29</sub>H<sub>25</sub>FN<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	37	29	1	4	3	0	0

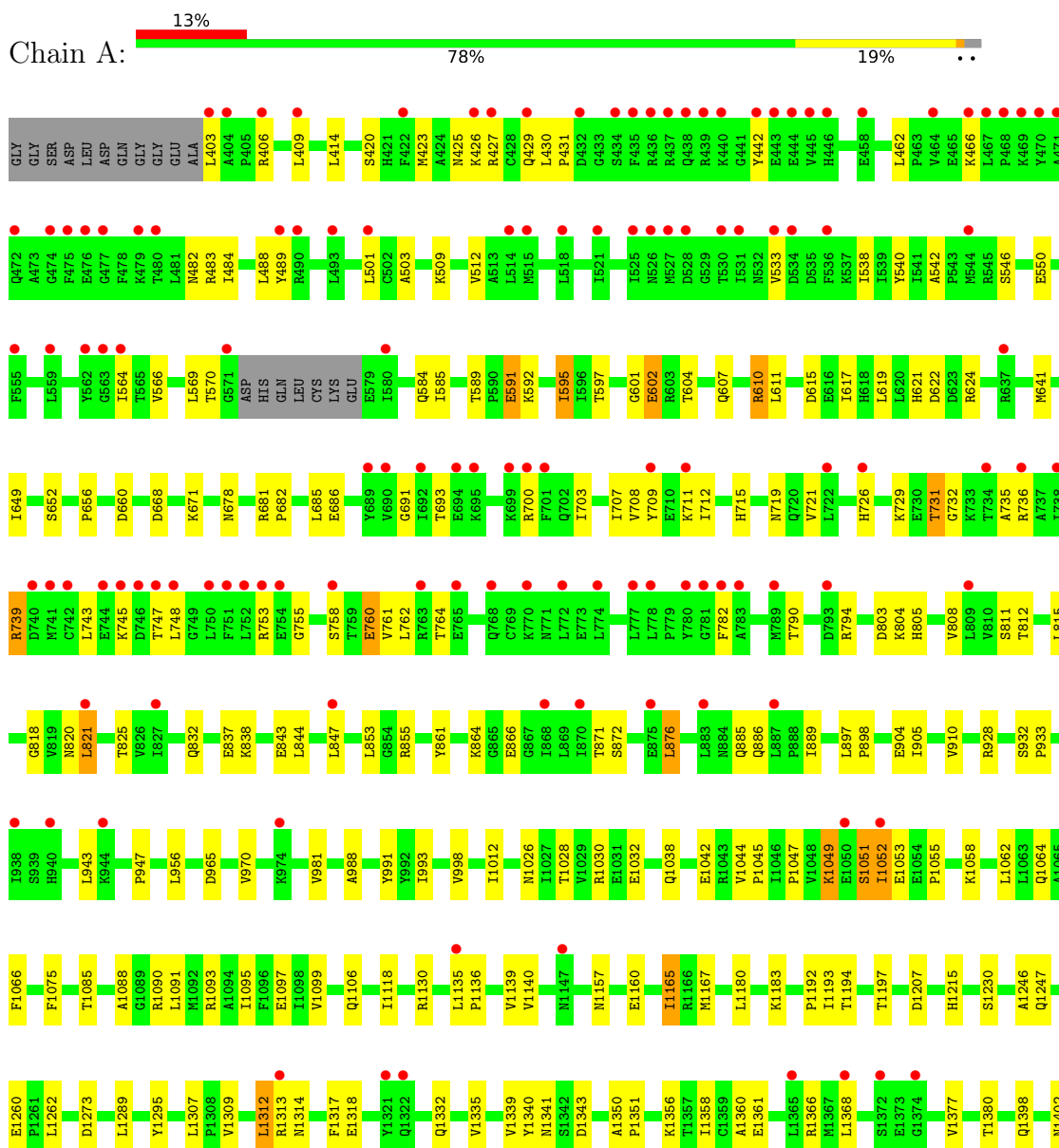
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		

### 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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.91Å 153.95Å 142.47Å 90.00° 120.50° 90.00°	Depositor
Resolution (Å)	48.46 – 2.75 48.46 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.46-2.75) 99.2 (48.46-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692, REFMAC	Depositor
R, $R_{free}$	0.237 , 0.286 0.241 , 0.288	Depositor DCC
$R_{free}$ test set	3498 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.1	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 64.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13745	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

### 5.1 Standard geometry

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

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	0.31	0/13976	0.51	3/18941 (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	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	876	LEU	CA-CB-CG	-5.77	102.03	115.30
1	A	821	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	1312	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1049	LYS	Peptide
1	A	2058	GLN	Peptide

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13688	0	13814	202	1
2	A	6	0	8	0	0
3	A	37	0	0	0	0
4	A	14	0	0	1	0
All	All	13745	0	13822	202	1

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 7.

All (202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:ARG:HG3	1:A:1140:VAL:HG11	1.70	0.73
1:A:1819:ALA:HB2	1:A:1829:ILE:HG12	1.72	0.72
1:A:815:LEU:HD21	1:A:821:LEU:HD11	1.72	0.71
1:A:423:MET:HE2	1:A:425:ASN:HB3	1.72	0.70
1:A:686:GLU:HG3	1:A:864:LYS:HD2	1.74	0.69
1:A:1994:ASN:HB2	1:A:1999:LEU:HD22	1.76	0.68
1:A:668:ASP:HB3	1:A:671:LYS:HB2	1.77	0.67
1:A:820:ASN:OD1	1:A:855:ARG:NH1	2.28	0.67
1:A:488:LEU:HD11	1:A:501:LEU:HD13	1.77	0.67
1:A:988:ALA:HB2	1:A:998:VAL:HG21	1.77	0.67
1:A:1341:ASN:O	1:A:1366:ARG:NH1	2.28	0.66
1:A:2013:ARG:HD3	1:A:2052:ILE:HD11	1.77	0.66
1:A:597:THR:HA	1:A:602:GLU:HB2	1.77	0.66
1:A:538:ILE:HB	1:A:585:ILE:HG13	1.76	0.66
1:A:1814:ASN:HA	1:A:1817:MET:HE2	1.77	0.66
1:A:1351:PRO:HG3	1:A:1516:PRO:HA	1.77	0.65
1:A:2023:VAL:HB	1:A:2026:LYS:HD2	1.78	0.65
1:A:566:VAL:HG22	1:A:585:ILE:HB	1.79	0.64
1:A:1246:ALA:O	1:A:1247:GLN:HB2	1.98	0.64
1:A:815:LEU:HD11	1:A:821:LEU:HD21	1.80	0.63
1:A:660:ASP:OD2	1:A:928:ARG:NH1	2.31	0.63
1:A:928:ARG:NH2	1:A:932:SER:OG	2.32	0.63
1:A:755:GLY:O	1:A:758:SER:N	2.32	0.62
1:A:1093:ARG:NH1	1:A:1273:ASP:OD1	2.32	0.62
1:A:617:ILE:HG22	1:A:652:SER:HB2	1.80	0.62
1:A:715:HIS:HB3	1:A:719:ASN:HB2	1.80	0.62
1:A:1358:ILE:HA	1:A:1361:GLU:HB2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1526:HIS:HB2	1:A:1703:VAL:HG22	1.81	0.61
1:A:1855:TYR:HB3	1:A:1891:THR:HG21	1.82	0.60
1:A:1456:VAL:HG22	1:A:1491:SER:HB2	1.82	0.60
1:A:753:ARG:NH1	1:A:764:THR:OG1	2.28	0.60
1:A:1939:ALA:C	1:A:1941:ALA:H	2.05	0.60
1:A:1049:LYS:O	1:A:1051:SER:N	2.34	0.60
1:A:1999:LEU:HD11	1:A:2004:ILE:HD11	1.83	0.60
1:A:1711:LYS:HG2	1:A:1715:LYS:HE2	1.85	0.59
1:A:1368:LEU:HD22	1:A:1403:LYS:HE2	1.85	0.58
1:A:1314:ASN:HB3	1:A:1317:PHE:HB2	1.85	0.57
1:A:1836:LEU:HD12	1:A:1930:LEU:HD21	1.85	0.57
1:A:1157:ASN:HB3	1:A:1160:GLU:OE1	2.06	0.56
1:A:1030:ARG:NH1	1:A:1032:GLU:OE2	2.39	0.56
1:A:1343:ASP:OD1	1:A:1366:ARG:NE	2.38	0.55
1:A:611:LEU:HD11	1:A:649:ILE:HD13	1.89	0.55
1:A:745:LYS:O	1:A:748:LEU:HG	2.07	0.54
1:A:2084:LEU:HD12	1:A:2085:GLN:H	1.71	0.54
1:A:1836:LEU:HD22	1:A:1848:ILE:HD13	1.90	0.54
1:A:758:SER:HA	1:A:761:VAL:HB	1.89	0.54
1:A:1666:THR:HG21	1:A:1714:PHE:CZ	2.43	0.54
1:A:703:ILE:O	1:A:707:ILE:HG12	2.09	0.53
1:A:2054:PRO:HG2	1:A:2055:LEU:HD12	1.90	0.53
1:A:905:ILE:HG22	1:A:981:VAL:HG22	1.91	0.53
1:A:2076:LEU:HD21	1:A:2079:ILE:HB	1.91	0.53
1:A:503:ALA:HB3	1:A:509:LYS:HE3	1.91	0.53
1:A:1561:VAL:HG22	1:A:1662:ILE:HB	1.90	0.53
1:A:832:GLN:NE2	1:A:843:GLU:OE1	2.41	0.53
1:A:1940:LEU:HD22	1:A:2109:MET:HE2	1.91	0.53
1:A:700:ARG:HH22	1:A:872:SER:HB3	1.73	0.52
1:A:1360:ALA:HB2	1:A:1490:LEU:HD11	1.90	0.52
1:A:1053:GLU:N	1:A:1053:GLU:OE1	2.43	0.52
1:A:753:ARG:HH11	1:A:761:VAL:HA	1.75	0.52
1:A:1183:LYS:HB3	1:A:1207:ASP:O	2.11	0.51
1:A:753:ARG:HH22	1:A:764:THR:HG21	1.74	0.51
1:A:790:THR:OG1	1:A:794:ARG:HG3	2.10	0.51
1:A:409:LEU:HD12	1:A:956:LEU:HD23	1.93	0.51
1:A:1604:LEU:HD21	1:A:1631:LEU:HD23	1.92	0.51
1:A:1648:ARG:HD2	1:A:1679:TYR:CE1	2.45	0.51
1:A:904:GLU:HB3	1:A:910:VAL:HG13	1.93	0.50
1:A:1456:VAL:CG2	1:A:1491:SER:HB2	2.42	0.50
1:A:607:GLN:O	1:A:610:ARG:NH2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1309:VAL:HG12	1:A:1318:GLU:HG2	1.94	0.50
1:A:1473:ARG:NH1	1:A:1739:GLU:OE2	2.44	0.50
1:A:1481:ILE:HG13	1:A:1483:ARG:H	1.77	0.50
1:A:1590:LEU:HD22	1:A:1614:LEU:O	2.11	0.50
1:A:641:MET:O	1:A:1578:THR:HB	2.12	0.49
1:A:429:GLN:O	1:A:886:GLN:NE2	2.45	0.49
1:A:1192:PRO:HG3	1:A:1289:LEU:HD11	1.93	0.49
1:A:1377:VAL:HG21	1:A:1432:TRP:CH2	2.46	0.49
1:A:550:GLU:HB2	1:A:818:GLY:O	2.12	0.49
1:A:1194:THR:OG1	1:A:1197:THR:HG22	2.13	0.49
1:A:1335:VAL:O	1:A:1339:VAL:HG12	2.13	0.49
1:A:1514:PHE:HB3	1:A:1518:VAL:HG21	1.94	0.48
1:A:700:ARG:NH2	1:A:872:SER:HB3	2.28	0.48
1:A:721:VAL:HG13	1:A:825:THR:HG23	1.95	0.48
1:A:1661:VAL:HG23	1:A:1691:ALA:HB2	1.96	0.48
1:A:569:LEU:O	1:A:592:LYS:HE2	2.14	0.48
1:A:691:GLY:HA2	1:A:871:THR:O	2.13	0.48
1:A:1667:GLN:HE21	1:A:1710:LYS:HE3	1.78	0.48
1:A:1088:ALA:HB1	1:A:1118:ILE:HD13	1.96	0.48
1:A:1617:VAL:HG22	1:A:1643:VAL:HB	1.95	0.47
1:A:1710:LYS:O	1:A:1713:PHE:HB3	2.14	0.47
1:A:1135:LEU:HD22	1:A:1140:VAL:HG23	1.95	0.47
1:A:1688:VAL:HG22	1:A:1702:CYS:SG	2.54	0.47
1:A:1095:ILE:O	1:A:1099:VAL:HG22	2.14	0.47
1:A:1165:ILE:HD12	1:A:1165:ILE:HA	1.72	0.47
1:A:1066:PHE:CG	1:A:1085:THR:HG21	2.49	0.47
1:A:1350:ALA:HB3	1:A:1356:LYS:HD3	1.96	0.47
1:A:707:ILE:O	1:A:711:LYS:HD3	2.15	0.47
1:A:708:VAL:O	1:A:712:ILE:HG12	2.14	0.47
1:A:1106:GLN:NE2	1:A:1230:SER:O	2.47	0.47
1:A:1398:GLN:O	1:A:1402:ASN:HA	2.14	0.47
1:A:760:GLU:HB3	1:A:805:HIS:HD1	1.80	0.47
1:A:570:THR:HG21	1:A:589:THR:HG23	1.97	0.47
1:A:1524:GLU:HB2	1:A:1701:ARG:HG2	1.97	0.47
1:A:681:ARG:HG3	1:A:682:PRO:HD2	1.96	0.47
1:A:484:ILE:HG22	1:A:488:LEU:HD12	1.97	0.46
1:A:1887:PRO:O	1:A:1891:THR:HG23	2.16	0.46
1:A:1970:HIS:HD2	1:A:1997:LEU:HD13	1.81	0.46
1:A:1351:PRO:CG	1:A:1516:PRO:HA	2.44	0.46
1:A:482:ASN:OD1	1:A:483:ARG:N	2.48	0.46
1:A:753:ARG:NH1	1:A:761:VAL:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:SER:HB2	1:A:762:LEU:HG	1.97	0.46
1:A:1351:PRO:HG2	1:A:1519:ARG:HB2	1.97	0.46
1:A:2019:LEU:HD12	1:A:2041:LEU:HD11	1.98	0.46
1:A:1538:ARG:NH2	4:A:2301:HOH:O	2.49	0.46
1:A:2051:VAL:HG13	1:A:2113:TYR:CZ	2.51	0.46
1:A:825:THR:HA	1:A:866:GLU:O	2.15	0.46
1:A:1577:LEU:HD22	1:A:1612:THR:HG22	1.97	0.45
1:A:1948:MET:HB2	1:A:1953:MET:O	2.15	0.45
1:A:712:ILE:HD13	1:A:721:VAL:HG11	1.98	0.45
1:A:2064:TRP:CZ3	1:A:2110:SER:HB2	2.50	0.45
1:A:1560:ILE:HG13	1:A:1658:ALA:HB2	1.98	0.45
1:A:782:PHE:HA	1:A:808:VAL:O	2.16	0.45
1:A:1136:PRO:HB2	1:A:1139:VAL:HG23	1.97	0.45
1:A:1398:GLN:HA	1:A:1403:LYS:O	2.16	0.45
1:A:1038:GLN:O	1:A:1042:GLU:HG2	2.17	0.45
1:A:1475:ARG:NH1	1:A:1505:GLY:HA3	2.31	0.45
1:A:619:LEU:HD13	1:A:847:LEU:HD22	1.99	0.44
1:A:430:LEU:HA	1:A:431:PRO:HD3	1.76	0.44
1:A:420:SER:HB2	1:A:622:ASP:HA	1.99	0.44
1:A:488:LEU:HD13	1:A:512:VAL:HG11	2.00	0.44
1:A:1883:LYS:HA	1:A:1883:LYS:HD3	1.84	0.44
1:A:1753:ASP:O	1:A:1756:THR:OG1	2.30	0.44
1:A:1028:THR:HA	1:A:1055:PRO:HG3	1.98	0.44
1:A:597:THR:HG22	1:A:602:GLU:HG3	1.98	0.44
1:A:726:HIS:CE1	1:A:844:LEU:HD22	2.53	0.44
1:A:731:THR:HG23	1:A:732:GLY:H	1.82	0.44
1:A:1193:ILE:HB	1:A:1197:THR:HG23	2.00	0.44
1:A:2096:ALA:HA	1:A:2097:PRO:HD3	1.69	0.44
1:A:803:ASP:HB2	1:A:805:HIS:CD2	2.53	0.43
1:A:1312:LEU:HD12	1:A:1340:TYR:CZ	2.53	0.43
1:A:564:ILE:HG23	1:A:584:GLN:HB2	2.00	0.43
1:A:933:PRO:HG3	1:A:943:LEU:HD22	2.00	0.43
1:A:965:ASP:HA	1:A:970:VAL:O	2.18	0.43
1:A:403:LEU:HA	1:A:406:ARG:HH21	1.82	0.43
1:A:837:GLU:O	1:A:1026:ASN:HB2	2.19	0.43
1:A:1879:LEU:HD12	1:A:1879:LEU:HA	1.74	0.43
1:A:1963:LEU:HD22	1:A:2007:VAL:HG13	2.00	0.43
1:A:681:ARG:NH1	1:A:685:LEU:HD22	2.34	0.43
1:A:542:ALA:O	1:A:589:THR:HA	2.19	0.43
1:A:540:TYR:OH	1:A:615:ASP:OD2	2.29	0.43
1:A:1498:LYS:HE3	1:A:1498:LYS:HB2	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:VAL:HG22	1:A:1167:MET:SD	2.58	0.43
1:A:753:ARG:HH12	1:A:764:THR:HG1	1.56	0.43
1:A:533:VAL:HG13	1:A:584:GLN:CD	2.40	0.42
1:A:409:LEU:HD13	1:A:414:LEU:HD11	2.00	0.42
1:A:1044:VAL:HA	1:A:1045:PRO:HD3	1.75	0.42
1:A:2084:LEU:HD12	1:A:2085:GLN:N	2.32	0.42
1:A:1058:LYS:O	1:A:1062:LEU:HG	2.19	0.42
1:A:1739:GLU:HB3	1:A:1744:THR:HB	2.02	0.42
1:A:2067:VAL:HG22	1:A:2079:ILE:HG13	2.01	0.42
1:A:1727:HIS:NE2	1:A:1770:TYR:OH	2.50	0.42
1:A:804:LYS:HE2	1:A:861:TYR:CE1	2.54	0.42
1:A:621:HIS:HB2	1:A:889:ILE:HG23	2.02	0.42
1:A:1091:LEU:O	1:A:1095:ILE:HG13	2.19	0.42
1:A:876:LEU:HA	1:A:876:LEU:HD23	1.55	0.42
1:A:1012:ILE:HG12	1:A:1047:PRO:O	2.20	0.42
1:A:1180:LEU:O	1:A:1215:HIS:NE2	2.49	0.42
1:A:1194:THR:H	1:A:1197:THR:HG23	1.84	0.42
1:A:442:TYR:HA	1:A:693:THR:HG23	2.02	0.41
1:A:466:LYS:HE3	1:A:466:LYS:HB3	1.94	0.41
1:A:591:GLU:OE1	1:A:624:ARG:NH2	2.38	0.41
1:A:595:ILE:HD13	1:A:595:ILE:HA	1.92	0.41
1:A:601:GLY:O	1:A:604:THR:HG22	2.21	0.41
1:A:811:SER:OG	1:A:812:THR:N	2.53	0.41
1:A:1404:LYS:HD3	1:A:1404:LYS:HA	1.81	0.41
1:A:426:LYS:HG3	1:A:427:ARG:H	1.85	0.41
1:A:678:ASN:H	1:A:885:GLN:HE22	1.68	0.41
1:A:905:ILE:HG12	1:A:910:VAL:HG22	2.01	0.41
1:A:736:ARG:HG3	1:A:739:ARG:HH22	1.85	0.41
1:A:1260:GLU:O	1:A:1262:LEU:N	2.52	0.41
1:A:1937:SER:HB2	1:A:1938:PRO:HD3	2.01	0.41
1:A:656:PRO:HD3	1:A:885:GLN:O	2.20	0.41
1:A:743:LEU:HA	1:A:747:THR:HA	2.02	0.41
1:A:871:THR:OG1	1:A:876:LEU:HD13	2.21	0.41
1:A:1886:ASP:HA	1:A:1887:PRO:HD2	1.95	0.41
1:A:709:TYR:CZ	1:A:748:LEU:HD13	2.56	0.41
1:A:729:LYS:HB3	1:A:1075:PHE:CE2	2.56	0.41
1:A:991:TYR:CE2	1:A:1097:GLU:HG3	2.56	0.41
1:A:1553:HIS:O	1:A:1701:ARG:NH1	2.50	0.41
1:A:1432:TRP:HE1	1:A:1474:MET:CE	2.34	0.40
1:A:1945:LEU:HA	1:A:1948:MET:HG2	2.04	0.40
1:A:2067:VAL:O	1:A:2106:LEU:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:LYS:HA	1:A:838:LYS:HD3	1.89	0.40
1:A:897:LEU:HB3	1:A:898:PRO:HD3	2.03	0.40
1:A:1332:GLN:CD	1:A:1358:ILE:HD11	2.41	0.40
1:A:1577:LEU:HD21	1:A:1612:THR:HA	2.03	0.40
1:A:758:SER:O	1:A:758:SER:OG	2.35	0.40
1:A:2031:SER:HA	1:A:2097:PRO:O	2.21	0.40
1:A:735:ALA:O	1:A:739:ARG:HB3	2.21	0.40
1:A:1295:TYR:CG	1:A:1495:SER:HB2	2.56	0.40
1:A:1692:ASN:ND2	1:A:1694:PRO:HD3	2.37	0.40
1:A:570:THR:HB	1:A:592:LYS:HG2	2.04	0.40
1:A:1044:VAL:HB	1:A:1064:GLN:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:PRO:O	1:A:1600:TYR:OH[2_557]	2.18	0.02

## 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	1699/1738 (98%)	1632 (96%)	62 (4%)	5 (0%)	41 60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1665	ASP
1	A	1940	LEU
1	A	1052	ILE
1	A	1584	ILE
1	A	1656	VAL

### 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	1520/1551 (98%)	1484 (98%)	36 (2%)	49 68

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	462	LEU
1	A	489	TYR
1	A	546	SER
1	A	591	GLU
1	A	595	ILE
1	A	602	GLU
1	A	610	ARG
1	A	731	THR
1	A	739	ARG
1	A	760	GLU
1	A	853	LEU
1	A	993	ILE
1	A	1051	SER
1	A	1052	ILE
1	A	1090	ARG
1	A	1165	ILE
1	A	1307	LEU
1	A	1313	ARG
1	A	1380	THR
1	A	1425	ILE
1	A	1480	GLN
1	A	1588	ARG
1	A	1637	SER
1	A	1649	SER
1	A	1656	VAL
1	A	1731	CYS
1	A	1842	VAL
1	A	1862	HIS
1	A	1879	LEU
1	A	1967	THR

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Mol	Chain	Res	Type
1	A	1991	GLU
1	A	1999	LEU
1	A	2000	THR
1	A	2058	GLN
1	A	2084	LEU
1	A	2099	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1069	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	GOL	A	2201	-	5,5,5	0.35	0	5,5,5	0.51	0
3	8LS	A	2202	-	41,42,42	1.28	5 (12%)	50,61,61	1.94	15 (30%)



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	GOL	A	2201	-	-	2/4/4/4	-
3	8LS	A	2202	-	-	0/11/49/49	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2202	8LS	C26-C24	-4.46	1.40	1.51
3	A	2202	8LS	C14-C27	-3.30	1.42	1.47
3	A	2202	8LS	C11-N12	-3.22	1.39	1.44
3	A	2202	8LS	C29-N12	-2.79	1.35	1.41
3	A	2202	8LS	C27-N28	2.01	1.39	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2202	8LS	C2-C11-N12	7.01	128.36	119.79
3	A	2202	8LS	C26-C24-N16	4.17	120.22	117.12
3	A	2202	8LS	C29-N28-C27	3.52	122.27	119.02
3	A	2202	8LS	C10-C11-N12	-3.49	111.30	118.86
3	A	2202	8LS	N12-C29-N28	2.90	123.34	119.57
3	A	2202	8LS	C36-C31-C7	-2.75	118.29	123.08
3	A	2202	8LS	C6-C5-C4	-2.66	107.82	112.87
3	A	2202	8LS	O30-C29-N28	-2.61	118.09	122.33
3	A	2202	8LS	C36-C31-N32	2.34	120.07	118.21
3	A	2202	8LS	C33-N32-C31	2.33	121.70	116.78
3	A	2202	8LS	C13-N12-C11	2.28	120.20	116.31
3	A	2202	8LS	C5-C4-C9	-2.26	118.39	120.36
3	A	2202	8LS	C18-C17-N16	-2.08	109.69	112.83
3	A	2202	8LS	C14-C27-N28	-2.06	119.96	123.29
3	A	2202	8LS	C26-C27-N28	2.02	121.59	117.06

There are no chirality outliers.

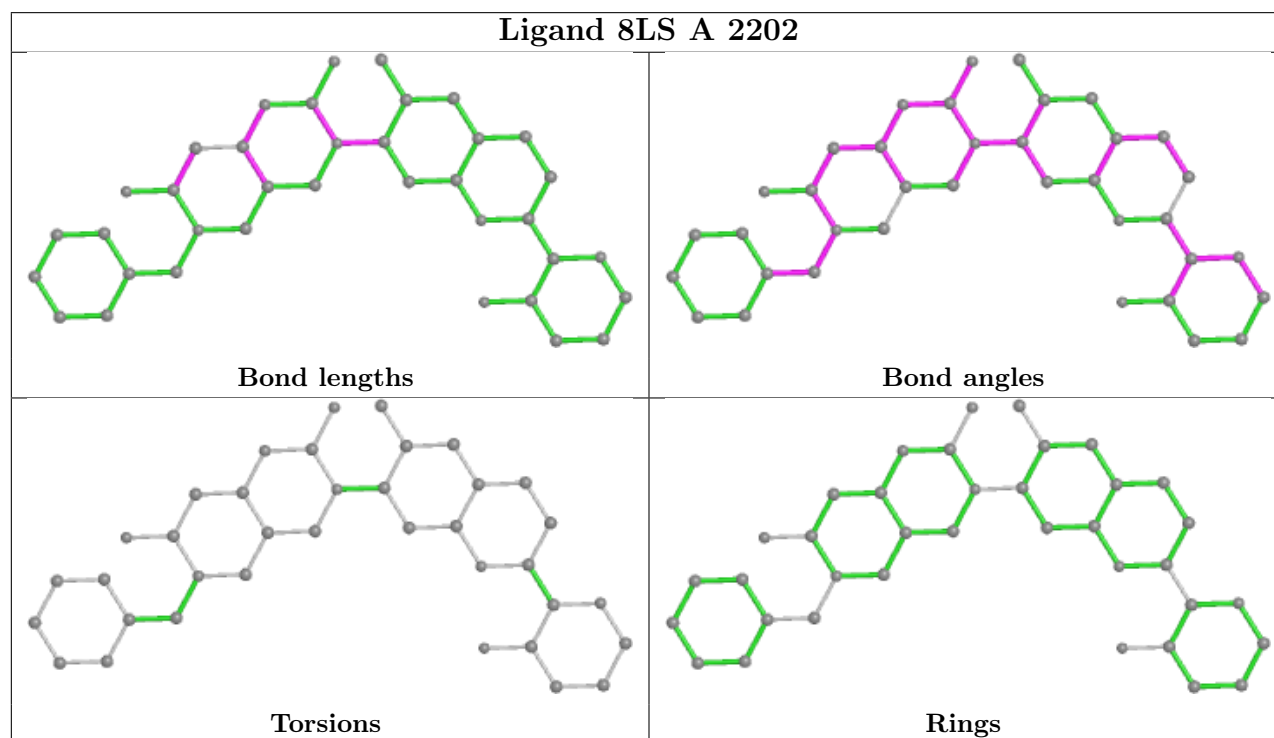
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2201	GOL	O1-C1-C2-C3
2	A	2201	GOL	O1-C1-C2-O2

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	A	1707/1738 (98%)	0.85	227 (13%) <b>3</b> <b>4</b>	55, 101, 161, 189	0

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	571	GLY	11.5
1	A	2004	ILE	10.5
1	A	746	ASP	10.1
1	A	2016	ASN	8.1
1	A	1982	VAL	8.1
1	A	2041	LEU	7.6
1	A	469	LYS	7.2
1	A	530	THR	6.9
1	A	1971	ILE	6.4
1	A	781	GLY	6.4
1	A	1973	ARG	6.4
1	A	1960	LEU	6.4
1	A	1983	PHE	6.3
1	A	763	ARG	6.3
1	A	2005	ALA	6.1
1	A	436	ARG	5.9
1	A	434	SER	5.7
1	A	1974	CYS	5.5
1	A	2052	ILE	5.5
1	A	2019	LEU	5.4
1	A	722	LEU	5.3
1	A	2047	VAL	5.3
1	A	2087	LYS	5.2
1	A	734	THR	5.1
1	A	525	ILE	5.1
1	A	527	MET	5.0
1	A	1976	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	875	GLU	5.0
1	A	479	LYS	5.0
1	A	2084	LEU	4.9
1	A	1963	LEU	4.8
1	A	1872	ALA	4.8
1	A	531	ILE	4.7
1	A	1050	GLU	4.7
1	A	694	GLU	4.7
1	A	474	GLY	4.6
1	A	2010	PHE	4.6
1	A	2122	PHE	4.6
1	A	736	ARG	4.5
1	A	526	ASN	4.5
1	A	464	VAL	4.5
1	A	2008	ALA	4.5
1	A	528	ASP	4.5
1	A	518	LEU	4.5
1	A	480	THR	4.4
1	A	809	LEU	4.4
1	A	741	MET	4.3
1	A	748	LEU	4.1
1	A	2006	ASP	4.1
1	A	1365	LEU	4.1
1	A	2104	TYR	4.1
1	A	2048	THR	4.1
1	A	637	ARG	4.1
1	A	564	ILE	4.1
1	A	821	LEU	4.0
1	A	1966	PHE	4.0
1	A	782	PHE	4.0
1	A	429	GLN	4.0
1	A	562	TYR	4.0
1	A	466	LYS	4.0
1	A	1970	HIS	3.9
1	A	689	TYR	3.9
1	A	437	ARG	3.9
1	A	2102	HIS	3.9
1	A	471	ALA	3.8
1	A	2085	GLN	3.8
1	A	1368	LEU	3.8
1	A	2049	GLY	3.8
1	A	427	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	726	HIS	3.8
1	A	536	PHE	3.8
1	A	2043	ARG	3.7
1	A	1372	SER	3.7
1	A	2003	GLN	3.7
1	A	2015	PRO	3.6
1	A	2002	SER	3.6
1	A	750	LEU	3.6
1	A	468	PRO	3.5
1	A	772	LEU	3.5
1	A	753	ARG	3.5
1	A	403	LEU	3.5
1	A	1991	GLU	3.5
1	A	2022	GLU	3.4
1	A	444	GLU	3.4
1	A	2035	VAL	3.4
1	A	2042	GLU	3.4
1	A	475	PHE	3.4
1	A	1997	LEU	3.4
1	A	1998	GLN	3.3
1	A	752	LEU	3.3
1	A	940	HIS	3.3
1	A	406	ARG	3.3
1	A	742	CYS	3.3
1	A	1981	SER	3.2
1	A	747	THR	3.2
1	A	2068	ILE	3.2
1	A	2038	LEU	3.2
1	A	2092	LEU	3.2
1	A	1313	ARG	3.2
1	A	1980	GLU	3.2
1	A	442	TYR	3.2
1	A	2088	ALA	3.2
1	A	477	GLY	3.2
1	A	555	PHE	3.2
1	A	2017	ILE	3.2
1	A	765	GLU	3.1
1	A	533	VAL	3.1
1	A	2012	ASN	3.1
1	A	974	LYS	3.1
1	A	2036	VAL	3.1
1	A	409	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1135	LEU	3.1
1	A	2082	LEU	3.1
1	A	1321	TYR	3.1
1	A	754	GLU	3.1
1	A	1969	GLU	3.1
1	A	1052	ILE	3.1
1	A	1322	GLN	3.1
1	A	758	SER	3.1
1	A	1421	LYS	3.1
1	A	514	LEU	3.0
1	A	439	ARG	3.0
1	A	2009	ARG	3.0
1	A	1873	GLN	3.0
1	A	1964	PRO	3.0
1	A	695	LYS	2.9
1	A	709	TYR	2.9
1	A	521	ILE	2.9
1	A	938	ILE	2.9
1	A	440	LYS	2.9
1	A	534	ASP	2.9
1	A	1975	THR	2.9
1	A	472	GLN	2.9
1	A	2120	TYR	2.9
1	A	699	LYS	2.9
1	A	2044	GLU	2.9
1	A	1871	LEU	2.9
1	A	2089	LYS	2.9
1	A	692	ILE	2.8
1	A	1604	LEU	2.8
1	A	1999	LEU	2.8
1	A	2079	ILE	2.8
1	A	780	TYR	2.8
1	A	563	GLY	2.8
1	A	2086	GLN	2.8
1	A	2013	ARG	2.8
1	A	432	ASP	2.7
1	A	2029	ILE	2.7
1	A	476	GLU	2.7
1	A	789	MET	2.7
1	A	2023	VAL	2.7
1	A	2062	GLU	2.7
1	A	2090	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	783	ALA	2.6
1	A	458	GLU	2.6
1	A	2106	LEU	2.6
1	A	1959	TYR	2.6
1	A	2113	TYR	2.6
1	A	1902	MET	2.6
1	A	445	VAL	2.6
1	A	690	VAL	2.5
1	A	493	LEU	2.5
1	A	774	LEU	2.5
1	A	2095	VAL	2.5
1	A	2098	ALA	2.5
1	A	2091	LYS	2.5
1	A	738	ILE	2.5
1	A	1940	LEU	2.4
1	A	438	GLN	2.4
1	A	944	LYS	2.4
1	A	559	LEU	2.4
1	A	2045	GLU	2.4
1	A	751	PHE	2.4
1	A	1883	LYS	2.4
1	A	887	LEU	2.4
1	A	711	LYS	2.4
1	A	1719	TYR	2.4
1	A	868	ILE	2.4
1	A	2067	VAL	2.4
1	A	2020	SER	2.4
1	A	580	ILE	2.4
1	A	740	ASP	2.4
1	A	870	ILE	2.4
1	A	883	LEU	2.3
1	A	443	GLU	2.3
1	A	1993	ARG	2.3
1	A	1429	PRO	2.3
1	A	467	LEU	2.3
1	A	1447	ASN	2.3
1	A	744	GLU	2.3
1	A	1147	ASN	2.2
1	A	544	MET	2.2
1	A	827	ILE	2.2
1	A	446	HIS	2.2
1	A	1880	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1881	ASN	2.2
1	A	2037	VAL	2.2
1	A	1952	ALA	2.2
1	A	489	TYR	2.2
1	A	1423	ASN	2.2
1	A	1403	LYS	2.2
1	A	470	TYR	2.1
1	A	404	ALA	2.1
1	A	1869	ARG	2.1
1	A	2026	LYS	2.1
1	A	1374	GLY	2.1
1	A	1990	ASP	2.1
1	A	2101	ALA	2.1
1	A	422	PHE	2.1
1	A	700	ARG	2.1
1	A	2094	PHE	2.1
1	A	847	LEU	2.1
1	A	777	LEU	2.1
1	A	2061	GLU	2.1
1	A	745	LYS	2.1
1	A	1954	TRP	2.1
1	A	490	ARG	2.1
1	A	793	ASP	2.1
1	A	770	LYS	2.0
1	A	778	LEU	2.0
1	A	768	GLN	2.0
1	A	501	LEU	2.0
1	A	435	PHE	2.0
1	A	515	MET	2.0
1	A	701	PHE	2.0
1	A	1482	GLU	2.0
1	A	426	LYS	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.

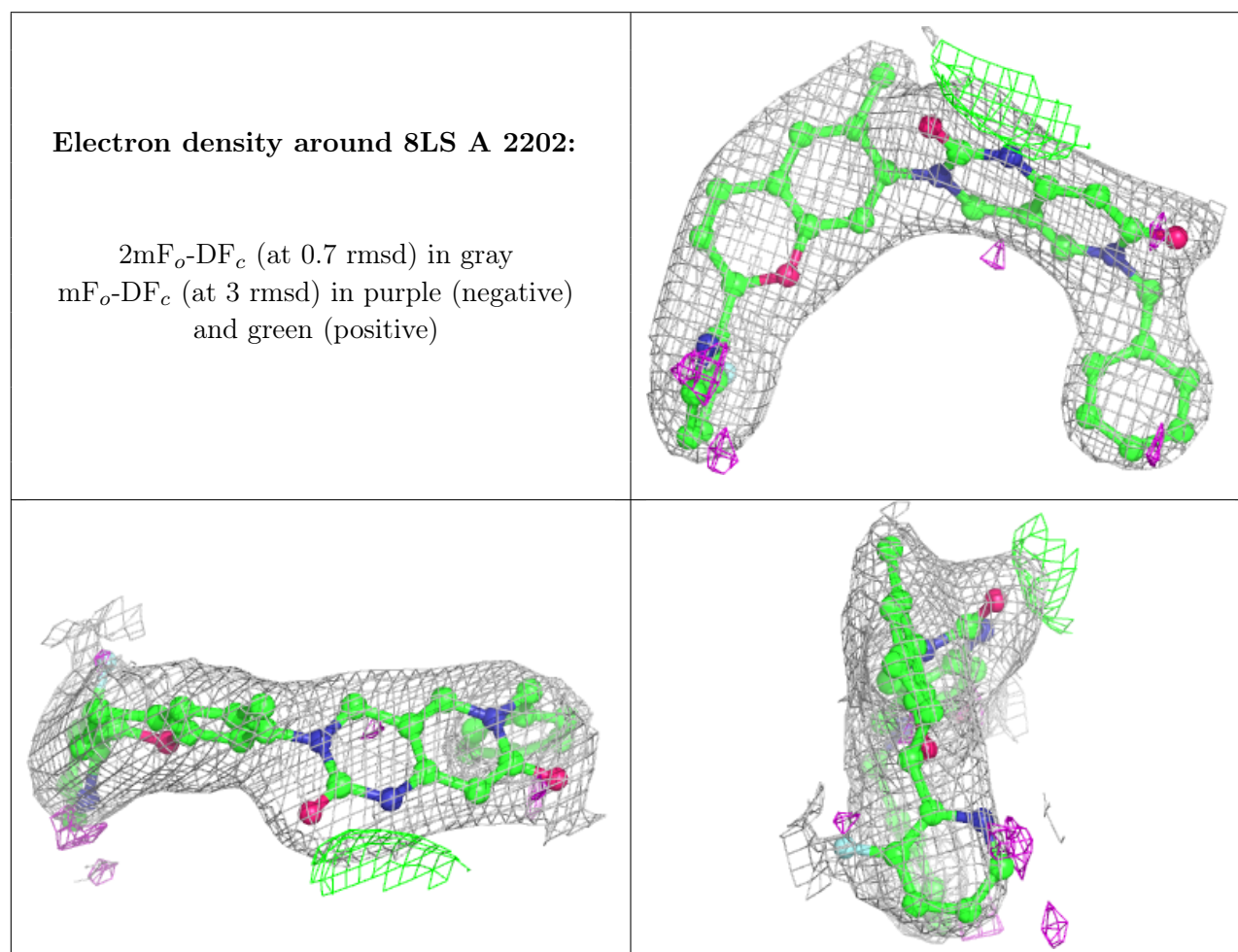


## 6.4 Ligands [i](#)

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, 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( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	2201	6/6	0.91	0.20	63,70,74,78	0
3	8LS	A	2202	37/37	0.95	0.19	60,67,83,86	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.