



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:48 PM UTC

PDB ID : 5URJ / pdb_00005urj
Title : Crystal structure of human BRR2 in complex with T-3905516
Authors : Klein, M.G.; Tjhen, R.; Qin, L.
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

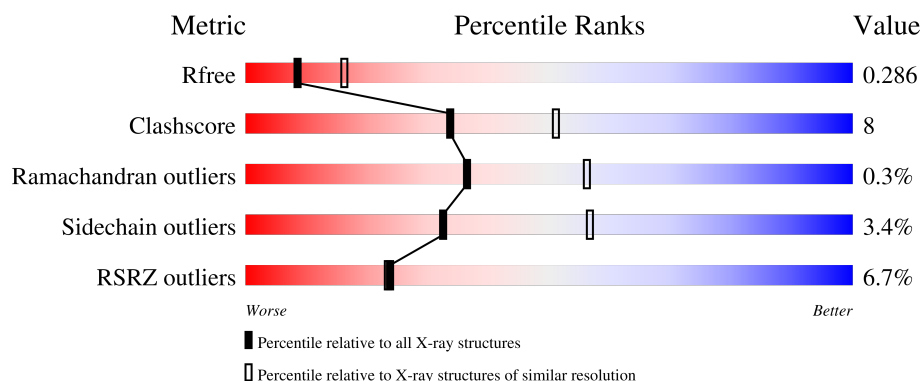
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1738	

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.

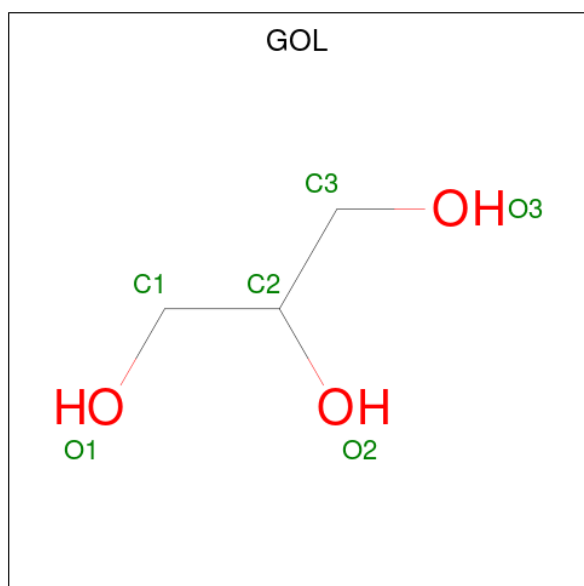
- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

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:

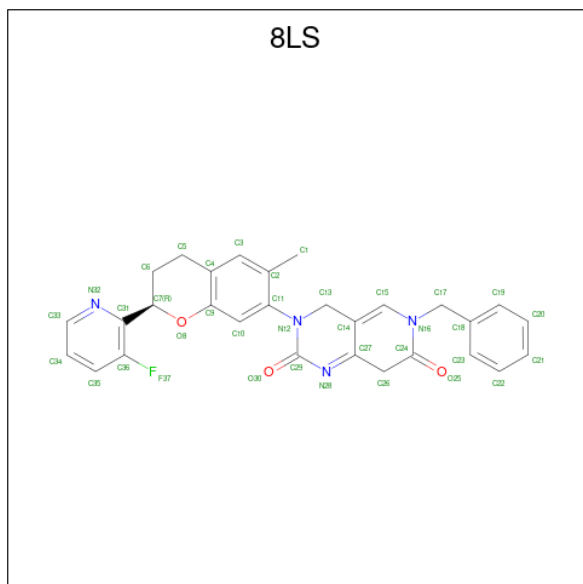
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	GLY	-	expression tag	UNP O75643
A	393	GLY	-	expression tag	UNP O75643
A	394	SER	-	expression tag	UNP O75643

- Molecule 2 is GLYCEROL (CCD ID: 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 (CCD ID: 8LS) (formula: $C_{29}H_{25}FN_4O_3$).



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

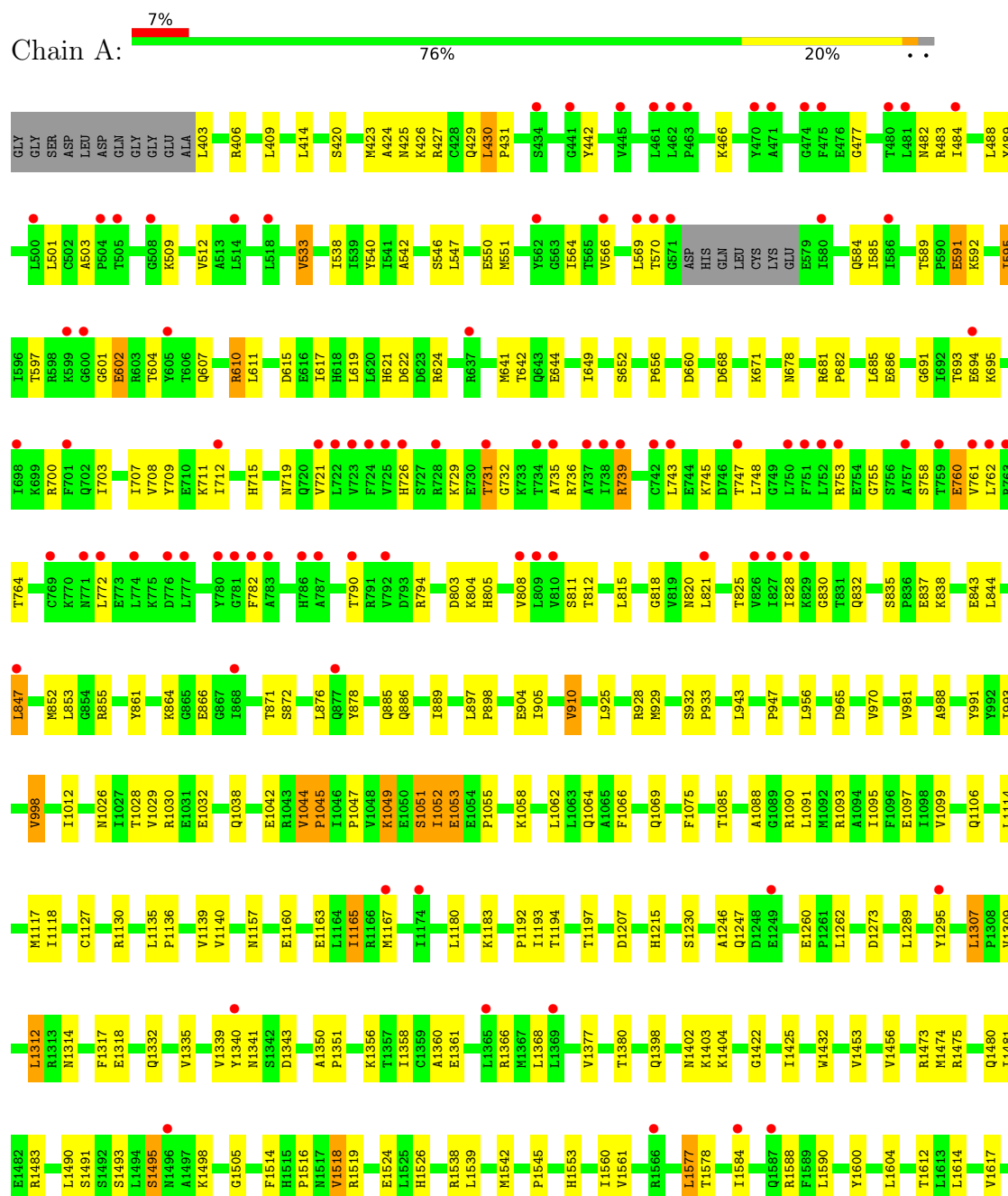
- Molecule 4 is water.

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

3 Residue-property plots

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692, REFMAC	Depositor
R, R_{free}	0.237 , 0.286 0.243 , 0.286	Depositor DCC
R_{free} test set	3505 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	87.1	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/13976	0.85	25/18941 (0.1%)

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 (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2096	ALA	CA-C-N	8.51	130.48	119.84
1	A	2096	ALA	C-N-CA	8.51	130.48	119.84
1	A	1044	VAL	CA-C-N	7.39	127.02	119.19
1	A	1044	VAL	C-N-CA	7.39	127.02	119.19
1	A	835	SER	CA-C-N	6.70	126.48	119.05
1	A	835	SER	C-N-CA	6.70	126.48	119.05
1	A	1732	MET	N-CA-C	6.43	119.98	111.75
1	A	1422	GLY	N-CA-C	5.85	119.22	111.03
1	A	1312	LEU	CA-C-N	-5.74	114.28	122.77
1	A	1312	LEU	C-N-CA	-5.74	114.28	122.77
1	A	2049	GLY	CA-C-N	5.67	126.92	119.84
1	A	2049	GLY	C-N-CA	5.67	126.92	119.84
1	A	1045	PRO	CA-C-N	-5.47	118.65	122.59
1	A	1045	PRO	C-N-CA	-5.47	118.65	122.59
1	A	424	ALA	N-CA-C	-5.41	106.64	113.18
1	A	830	GLY	N-CA-C	5.36	122.22	114.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	GLY	N-CA-C	-5.35	108.33	114.69
1	A	430	LEU	CA-C-N	5.24	125.40	119.90
1	A	430	LEU	C-N-CA	5.24	125.40	119.90
1	A	1127	CYS	CA-C-N	5.22	125.52	119.47
1	A	1127	CYS	C-N-CA	5.22	125.52	119.47
1	A	772	LEU	CB-CA-C	-5.20	109.06	116.34
1	A	1495	SER	N-CA-C	-5.15	105.75	111.36
1	A	1307	LEU	CA-C-N	5.12	125.33	120.31
1	A	1307	LEU	C-N-CA	5.12	125.33	120.31

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13688	0	13814	212	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	212	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 8.

All (212) 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:1940:LEU:HB3	1:A:2109:MET:HE3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:423:MET:HE2	1:A:425:ASN:HB3	1.76	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: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:1939:ALA:C	1:A:1941:ALA:H	2.05	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:1814:ASN:HA	1:A:1817:MET:HE2	1.79	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
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: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:1432:TRP:HE1	1:A:1474:MET:HE3	1.66	0.59
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:828:ILE:HD13	1:A:852:MET:HE3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1493:SER:OG	1:A:1514:PHE:O	2.23	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: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:OE1	1:A:1053:GLU:N	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
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:1953:MET:HE2	1:A:2114:MET:HE2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1114:LEU:HA	1:A:1117:MET:HE3	1.95	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:533:VAL:HG13	1:A:584:GLN:CD	2.40	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:1753:ASP:O	1:A:1756:THR:OG1	2.30	0.46
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1332:GLN:CD	1:A:1358:ILE:HD11	2.41	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:642:THR:C	1:A:644:GLU:H	2.24	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:540:TYR:OH	1:A:615:ASP:OD2	2.29	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:547:LEU:HD11	1:A:551:MET:HE2	1.99	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:1498:LYS:HE3	1:A:1498:LYS:HB2	1.79	0.43
1:A:1139:VAL:HG22	1:A:1167:MET:SD	2.58	0.43
1:A:1627:MET:HE3	1:A:1627:MET:HB3	1.93	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:1806:ASP:C	1:A:1808:MET:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1542:MET:C	1:A:1545:PRO:HD2	2.45	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:925:LEU:HG	1:A:929:MET:HE2	2.02	0.41
1:A:1404:LYS:HA	1:A:1404:LYS:HD3	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:876:LEU:C	1:A:878:TYR:N	2.79	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36 56

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%)	1469 (97%)	51 (3%)	32 57

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	489	TYR
1	A	533	VAL
1	A	546	SER
1	A	591	GLU
1	A	595	ILE
1	A	602	GLU
1	A	610	ARG
1	A	694	GLU
1	A	695	LYS
1	A	731	THR
1	A	739	ARG
1	A	760	GLU
1	A	847	LEU
1	A	853	LEU
1	A	910	VAL
1	A	993	ILE
1	A	998	VAL
1	A	1029	VAL
1	A	1051	SER
1	A	1052	ILE
1	A	1053	GLU
1	A	1069	GLN
1	A	1090	ARG
1	A	1163	GLU
1	A	1165	ILE
1	A	1307	LEU
1	A	1380	THR
1	A	1425	ILE
1	A	1453	VAL
1	A	1480	GLN
1	A	1518	VAL
1	A	1539	LEU
1	A	1577	LEU
1	A	1588	ARG

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Mol	Chain	Res	Type
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	1878	LYS
1	A	1879	LEU
1	A	1967	THR
1	A	1991	GLU
1	A	1999	LEU
1	A	2000	THR
1	A	2058	GLN
1	A	2077	ILE
1	A	2084	LEU
1	A	2090	VAL
1	A	2099	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	584	GLN
1	A	719	ASN
1	A	720	GLN
1	A	884	ASN
1	A	951	GLN
1	A	1069	GLN
1	A	1175	HIS
1	A	1189	HIS
1	A	1502	HIS
1	A	1531	ASN
1	A	1778	HIS
1	A	1951	GLN
1	A	2118	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	8LS	A	2202	-	41,42,42	1.89	6 (14%)	48,61,61	2.00	14 (29%)
2	GOL	A	2201	-	5,5,5	0.36	0	5,5,5	0.55	0

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
3	8LS	A	2202	-	-	1/12/49/49	0/6/6/6
2	GOL	A	2201	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2202	8LS	C26-C27	-8.71	1.39	1.50
3	A	2202	8LS	C26-C24	-4.54	1.40	1.51
3	A	2202	8LS	C11-N12	-3.43	1.39	1.44
3	A	2202	8LS	C14-C27	-3.42	1.42	1.47
3	A	2202	8LS	C29-N12	-2.84	1.35	1.41
3	A	2202	8LS	C27-N28	2.04	1.39	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2202	8LS	C2-C11-N12	7.51	128.36	119.78
3	A	2202	8LS	C26-C24-N16	4.24	120.22	117.12
3	A	2202	8LS	C10-C11-N12	-3.80	111.30	119.17
3	A	2202	8LS	C29-N28-C27	3.60	122.27	119.02
3	A	2202	8LS	C36-C31-C7	-3.06	118.29	123.07
3	A	2202	8LS	O30-C29-N28	-2.69	118.09	122.33
3	A	2202	8LS	C6-C5-C4	-2.66	107.82	112.87
3	A	2202	8LS	N12-C29-N28	2.54	123.34	119.16
3	A	2202	8LS	C14-C15-N16	-2.53	120.33	123.56
3	A	2202	8LS	C36-C31-N32	2.50	120.07	118.09
3	A	2202	8LS	C33-N32-C31	2.40	121.70	116.92
3	A	2202	8LS	C5-C4-C9	-2.27	118.39	120.35
3	A	2202	8LS	C14-C27-N28	-2.23	119.96	123.32
3	A	2202	8LS	C18-C17-N16	-2.04	109.69	112.84

There are no chirality outliers.

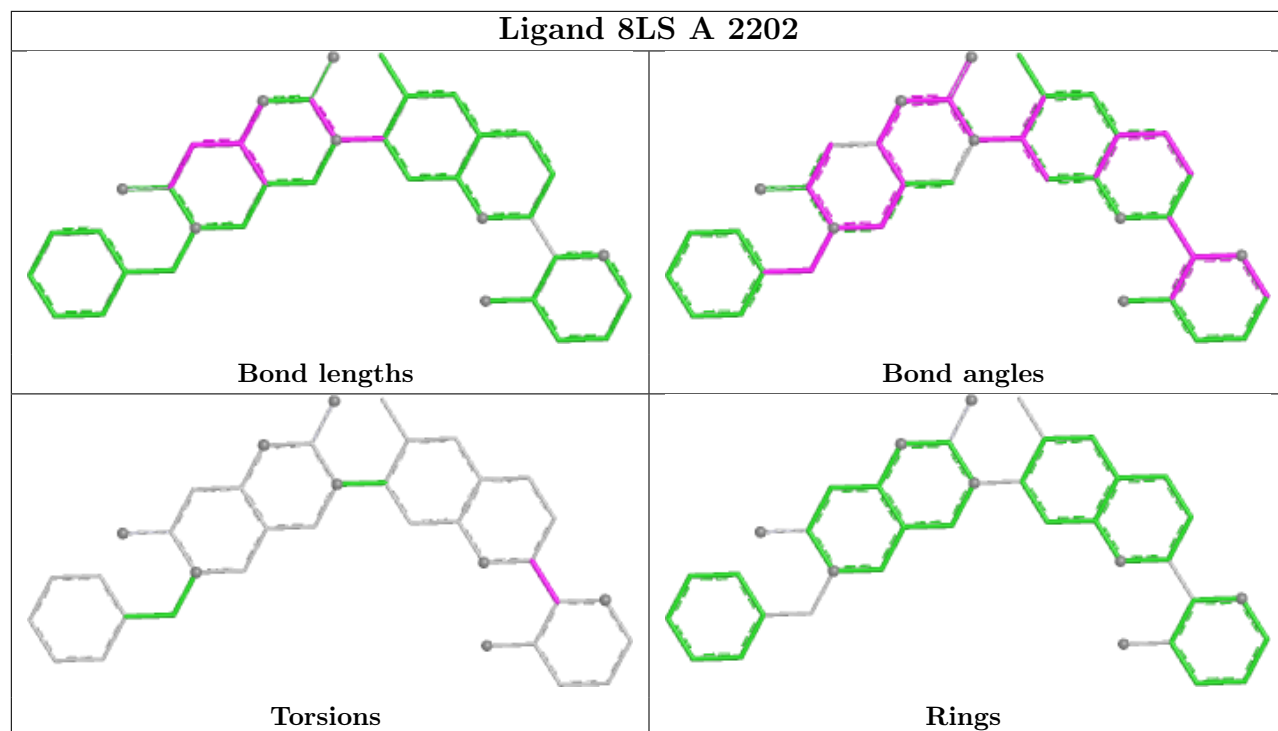
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2201	GOL	O1-C1-C2-C3
3	A	2202	8LS	N32-C31-C7-O8
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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1707/1738 (98%)	0.62	114 (6%)	24 23	55, 101, 161, 189	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	580	ILE	6.7
1	A	735	ALA	6.4
1	A	722	LEU	5.4
1	A	781	GLY	4.8
1	A	743	LEU	4.4
1	A	783	ALA	3.9
1	A	1966	PHE	3.8
1	A	777	LEU	3.8
1	A	782	PHE	3.8
1	A	739	ARG	3.7
1	A	821	LEU	3.7
1	A	752	LEU	3.5
1	A	809	LEU	3.5
1	A	637	ARG	3.5
1	A	1369	LEU	3.4
1	A	738	ILE	3.4
1	A	753	ARG	3.4
1	A	2100	GLY	3.3
1	A	2004	ILE	3.3
1	A	787	ALA	3.2
1	A	772	LEU	3.2
1	A	1584	ILE	3.1
1	A	712	ILE	3.1
1	A	1996	LEU	3.0
1	A	480	THR	3.0
1	A	762	LEU	3.0
1	A	877	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	828	ILE	3.0
1	A	571	GLY	2.9
1	A	724	PHE	2.9
1	A	868	ILE	2.9
1	A	461	LEU	2.9
1	A	728	ARG	2.9
1	A	780	TYR	2.9
1	A	827	ILE	2.9
1	A	731	THR	2.9
1	A	474	GLY	2.9
1	A	1960	LEU	2.9
1	A	2005	ALA	2.9
1	A	751	PHE	2.9
1	A	569	LEU	2.8
1	A	2035	VAL	2.8
1	A	1974	CYS	2.7
1	A	500	LEU	2.7
1	A	518	LEU	2.7
1	A	734	THR	2.7
1	A	808	VAL	2.7
1	A	2084	LEU	2.6
1	A	737	ALA	2.6
1	A	721	VAL	2.6
1	A	774	LEU	2.6
1	A	2041	LEU	2.6
1	A	726	HIS	2.6
1	A	829	LYS	2.6
1	A	1496	ASN	2.6
1	A	434	SER	2.5
1	A	586	ILE	2.5
1	A	2052	ILE	2.5
1	A	1997	LEU	2.5
1	A	605	TYR	2.5
1	A	810	VAL	2.5
1	A	1587	GLN	2.5
1	A	694	GLU	2.5
1	A	786	HIS	2.5
1	A	747	THR	2.5
1	A	514	LEU	2.4
1	A	1365	LEU	2.4
1	A	508	GLY	2.4
1	A	742	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	462	LEU	2.4
1	A	505	THR	2.4
1	A	771	ASN	2.3
1	A	599	LYS	2.3
1	A	504	PRO	2.3
1	A	1566	ARG	2.3
1	A	445	VAL	2.3
1	A	723	VAL	2.3
1	A	1249	GLU	2.3
1	A	759	THR	2.3
1	A	763	ARG	2.3
1	A	750	LEU	2.3
1	A	1940	LEU	2.3
1	A	792	VAL	2.3
1	A	847	LEU	2.3
1	A	1174	ILE	2.2
1	A	1340	TYR	2.2
1	A	470	TYR	2.2
1	A	776	ASP	2.2
1	A	761	VAL	2.2
1	A	790	THR	2.2
1	A	562	TYR	2.2
1	A	2104	TYR	2.2
1	A	475	PHE	2.2
1	A	1985	ILE	2.2
1	A	600	GLY	2.2
1	A	2023	VAL	2.2
1	A	769	CYS	2.1
1	A	1295	TYR	2.1
1	A	471	ALA	2.1
1	A	481	LEU	2.1
1	A	2016	ASN	2.1
1	A	441	GLY	2.1
1	A	698	ILE	2.1
1	A	725	VAL	2.1
1	A	826	VAL	2.1
1	A	701	PHE	2.1
1	A	757	ALA	2.1
1	A	570	THR	2.1
1	A	2106	LEU	2.1
1	A	484	ILE	2.1
1	A	566	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1982	VAL	2.1
1	A	1167	MET	2.0
1	A	463	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

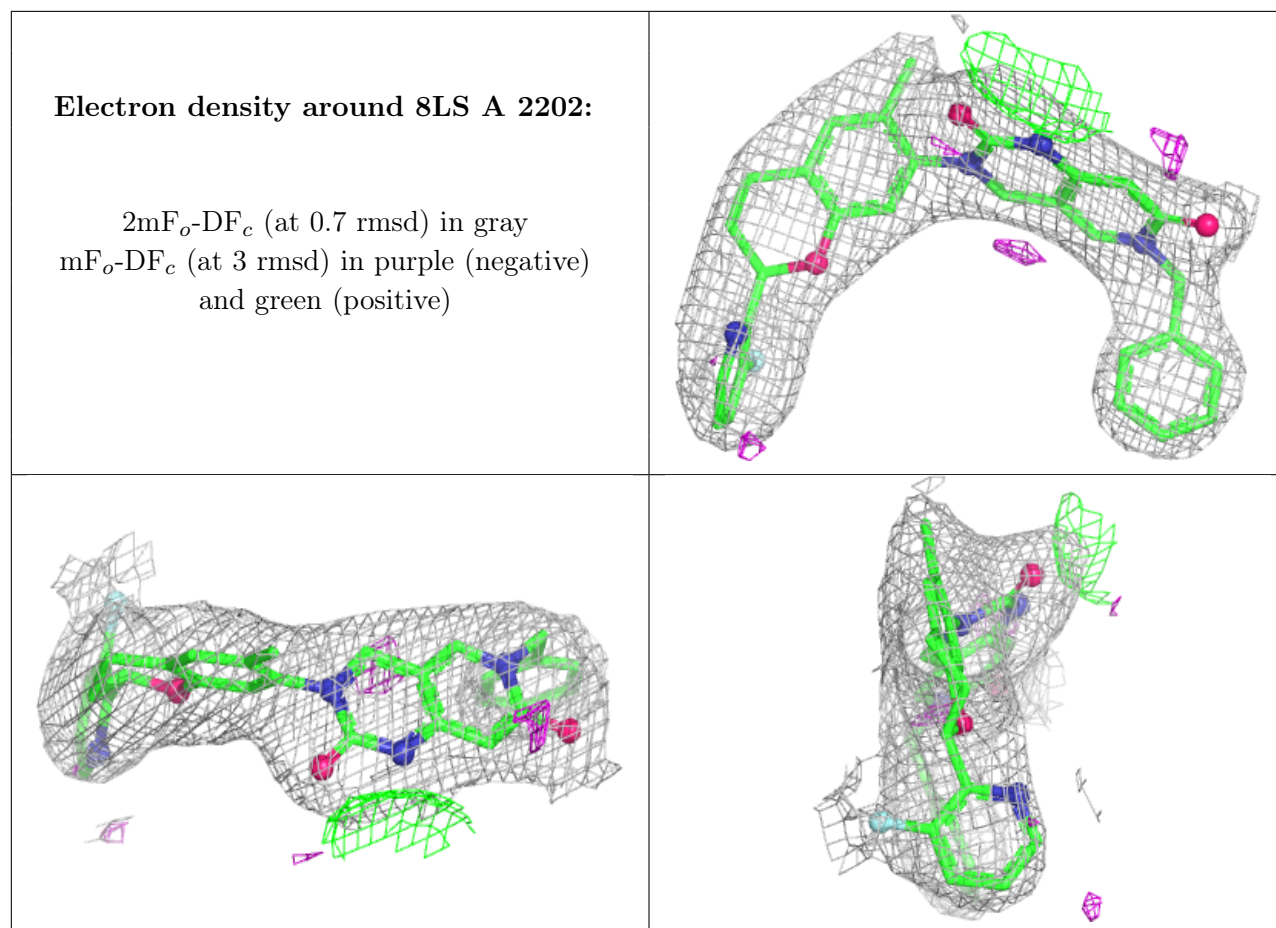
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	2201	6/6	0.88	0.14	63,70,74,78	0
3	8LS	A	2202	37/37	0.94	0.09	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 ⓘ

There are no such residues in this entry.