



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:50 PM UTC

PDB ID : 8BCC / pdb\_00008bcc  
Title : Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and compound 39  
Authors : Vester, K.; Loll, B.; Wahl, M.C.  
Deposited on : 2022-10-15  
Resolution : 2.35 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)  
Xtrriage (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

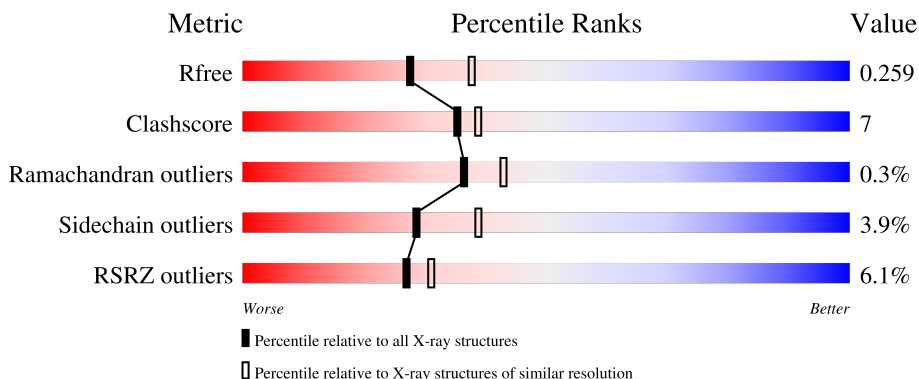
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	J	263	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 16497 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	1725	13879	8870	2375	2562	72	0	1	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

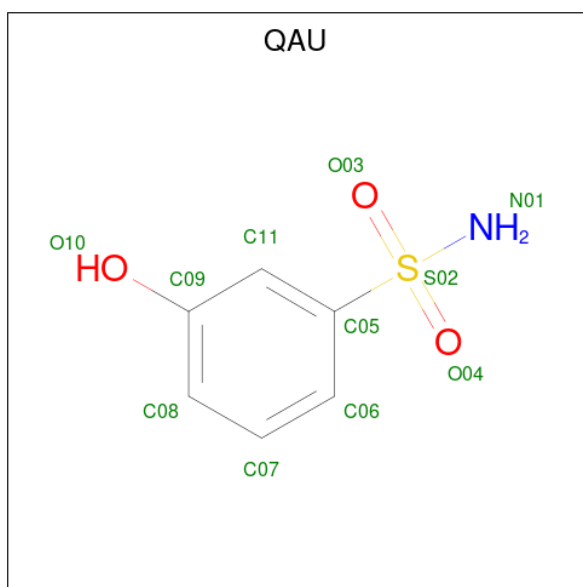
- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	263	2123	1358	365	388	12	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	2058	GLY	-	expression tag	UNP Q6P2Q9
J	2059	PRO	-	expression tag	UNP Q6P2Q9
J	2060	LEU	-	expression tag	UNP Q6P2Q9
J	2061	GLY	-	expression tag	UNP Q6P2Q9
J	2062	SER	-	expression tag	UNP Q6P2Q9
J	2063	MET	-	expression tag	UNP Q6P2Q9

- Molecule 3 is 3-oxidanylbenzenesulfonamide (CCD ID: QAU) (formula: C<sub>6</sub>H<sub>7</sub>NO<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	B	1	Total	C	N	O	S	0	0
			11	6	1	3	1		
3	B	1	Total	C	N	O	S	0	0
			11	6	1	3	1		
3	B	1	Total	C	N	O	S	0	0
			11	6	1	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

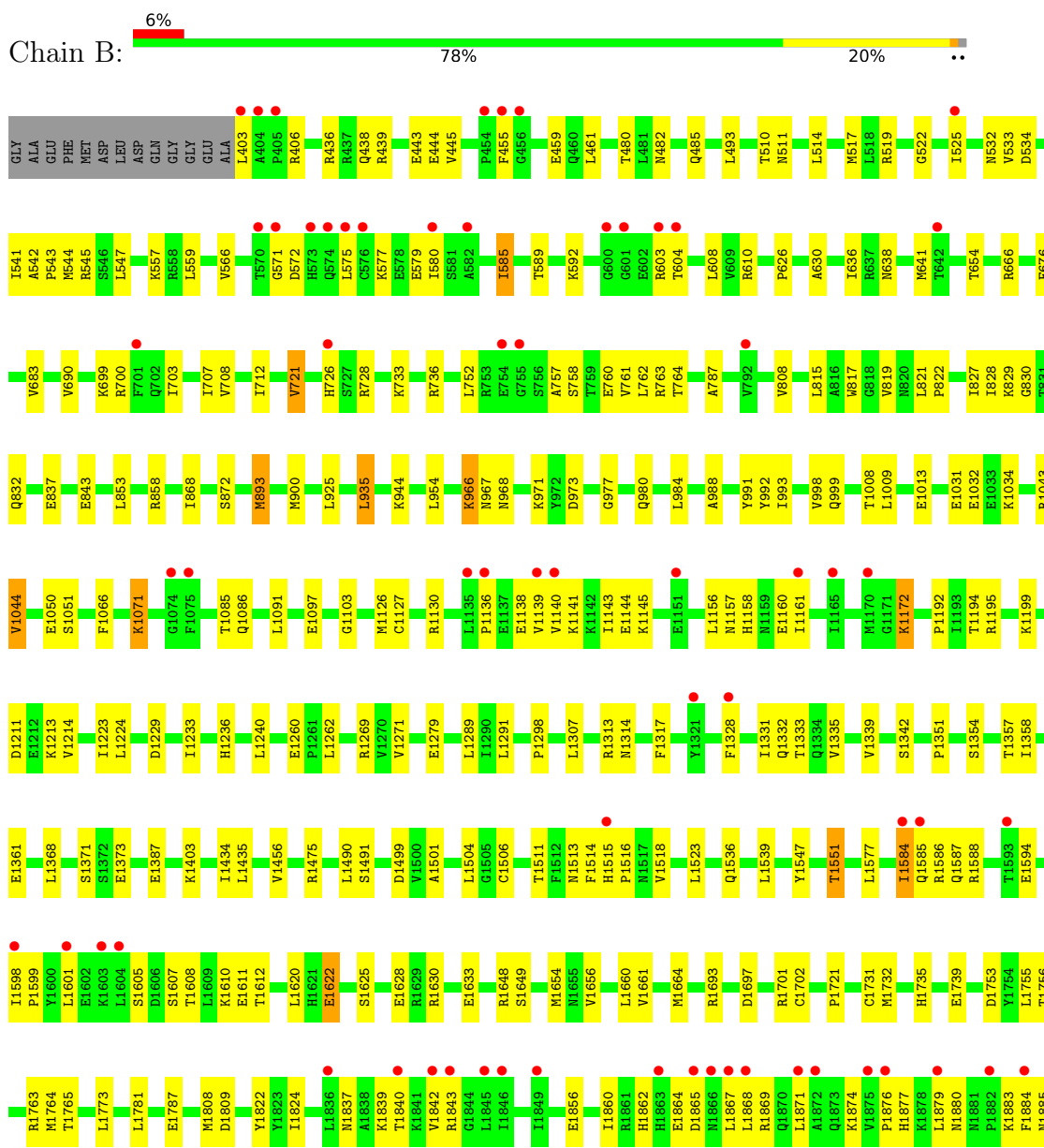
- Molecule 5 is water.

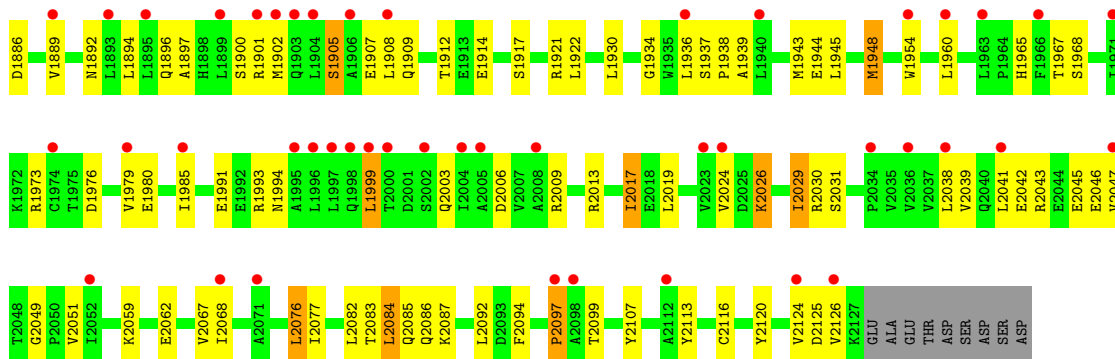
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	355	Total O 355 355	0	0
5	J	67	Total O 67 67	0	0

### 3 Residue-property plots [i](#)

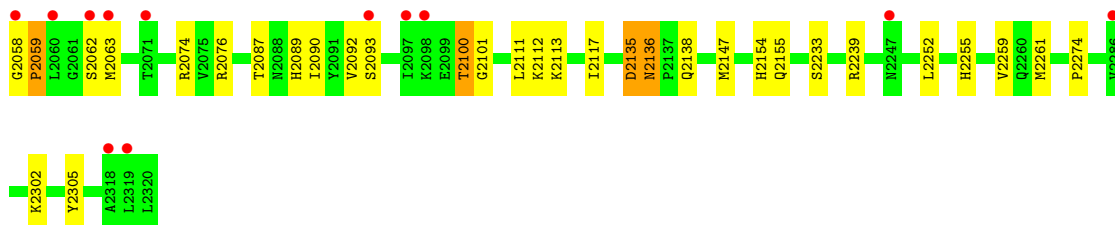
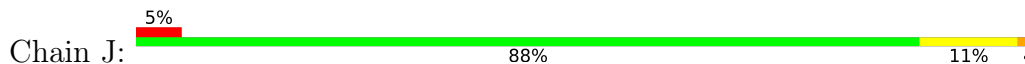
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: U5 small nuclear ribonucleoprotein 200 kDa helicase





• Molecule 2: Pre-mRNA-processing-splicing factor 8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.42Å 119.41Å 188.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 2.35 48.61 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.61-2.35) 99.8 (48.61-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, $R_{free}$	0.210 , 0.258 0.210 , 0.259	Depositor DCC
$R_{free}$ test set	2100 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 33.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: QAU, EDO

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	0.27	0/14173	0.47	0/19203
2	J	0.27	0/2190	0.47	0/2981
All	All	0.27	0/16363	0.47	0/22184

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	13879	0	14025	220	0
2	J	2123	0	2063	19	0
3	B	33	0	0	1	0
4	B	40	0	60	4	0
5	B	355	0	0	7	0
5	J	67	0	0	2	0
All	All	16497	0	16148	237	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 7.

All (237) 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:1351:PRO:HG3	1:B:1516:PRO:HA	1.62	0.81
1:B:511:ASN:ND2	5:B:5902:HOH:O	2.14	0.80
1:B:2043:ARG:HB3	1:B:2086:GLN:HA	1.63	0.80
1:B:893:MET:HG2	1:B:925:LEU:HD22	1.63	0.79
1:B:603:ARG:HD2	1:B:1862:HIS:HB2	1.65	0.79
1:B:760:GLU:HG3	1:B:763:ARG:HH12	1.48	0.78
1:B:1199:LYS:NZ	5:B:5905:HOH:O	2.20	0.74
1:B:1994:ASN:HB3	1:B:1999:LEU:HD22	1.69	0.73
1:B:1539:LEU:HD22	1:B:1664:MET:HE3	1.71	0.73
1:B:436:ARG:HG3	1:B:445:VAL:HG22	1.71	0.72
1:B:1900:SER:HB2	1:B:1954:TRP:HE1	1.52	0.72
1:B:1732:MET:HE1	1:B:1755:LEU:HD21	1.72	0.71
1:B:1298:PRO:HB3	1:B:1515:HIS:CG	2.26	0.70
1:B:1894:LEU:HB3	1:B:1912:THR:HG22	1.74	0.69
1:B:993:ILE:HD12	1:B:1091:LEU:HD23	1.74	0.69
1:B:532:ASN:O	1:B:534:ASP:N	2.19	0.68
2:J:2302:LYS:NZ	5:J:2401:HOH:O	2.26	0.67
1:B:1156:LEU:HB3	1:B:1160:GLU:HB2	1.78	0.66
1:B:482:ASN:OD1	1:B:485:GLN:NE2	2.25	0.66
1:B:1585:GLN:HB3	1:B:1588:ARG:HD2	1.79	0.65
1:B:1979:VAL:HG21	1:B:1993:ARG:HH12	1.62	0.65
2:J:2092:VAL:HG13	2:J:2261:MET:HE3	1.77	0.65
1:B:1501:ALA:HB1	1:B:1506:CYS:HB2	1.80	0.64
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	1.79	0.64
1:B:1475:ARG:HD2	1:B:1504:LEU:HA	1.79	0.64
1:B:461:LEU:HB3	1:B:480:THR:HG21	1.79	0.64
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	1.80	0.64
1:B:991:TYR:OH	1:B:1097:GLU:OE1	2.12	0.62
1:B:1009:LEU:HD22	1:B:1013:GLU:HG2	1.81	0.62
1:B:1908:LEU:HD12	1:B:1908:LEU:H	1.64	0.62
1:B:1900:SER:O	1:B:1902:MET:N	2.33	0.61
1:B:1874:LYS:HD3	1:B:1902:MET:HE1	1.83	0.61
1:B:1044:VAL:O	2:J:2074:ARG:NH1	2.32	0.60
1:B:1860:ILE:HG21	1:B:1885:ASN:HD22	1.65	0.60
1:B:2043:ARG:NH2	1:B:2084:LEU:O	2.34	0.59
1:B:514:LEU:HD12	1:B:517:MET:HE2	1.83	0.59
1:B:577:LYS:HA	1:B:580:ILE:HD13	1.85	0.58
1:B:1967:THR:HG22	1:B:1968:SER:H	1.68	0.58
1:B:1864:GLU:O	1:B:1868:LEU:N	2.25	0.58
1:B:2067:VAL:HB	1:B:2107:TYR:HB2	1.85	0.58
1:B:1194:THR:HB	4:B:5809:EDO:H21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1622:GLU:CD	1:B:1622:GLU:H	2.12	0.57
2:J:2087:THR:HB	2:J:2112:LYS:HG2	1.86	0.57
1:B:1965:HIS:ND1	1:B:2003:GLN:HB3	2.19	0.57
1:B:1843:ARG:HB3	1:B:1877:HIS:ND1	2.19	0.57
1:B:1884:PHE:HD1	1:B:1885:ASN:H	1.52	0.57
1:B:2051:VAL:HG22	1:B:2062:GLU:HG2	1.85	0.56
1:B:708:VAL:HG21	1:B:829:LYS:HD2	1.87	0.56
1:B:1594:GLU:O	1:B:1598:ILE:HG12	2.06	0.56
1:B:2006:ASP:O	1:B:2009:ARG:HG2	2.05	0.56
1:B:1586:ARG:HD2	1:B:1587:GLN:H	1.71	0.55
1:B:1314:ASN:HB3	1:B:1317:PHE:HB2	1.88	0.55
1:B:2125:ASP:OD1	1:B:2126:VAL:N	2.40	0.55
1:B:752:LEU:HD21	1:B:762:LEU:HD12	1.89	0.55
1:B:1043:ARG:HA	2:J:2074:ARG:NH2	2.22	0.55
1:B:2024:VAL:HG22	1:B:2038:LEU:HD23	1.89	0.55
1:B:1765:THR:HG22	1:B:1781:LEU:HD21	1.87	0.54
1:B:1513:ASN:OD1	5:B:5903:HOH:O	2.18	0.54
1:B:636:ILE:HD13	1:B:666:ARG:HD2	1.89	0.54
1:B:654:THR:HG21	1:B:676:PHE:O	2.07	0.54
1:B:1515:HIS:NE2	1:B:1721:PRO:HG3	2.23	0.54
1:B:2026:LYS:HB3	1:B:2124:VAL:HG11	1.88	0.54
1:B:1127:CYS:HB2	1:B:1144:GLU:HG2	1.89	0.54
1:B:461:LEU:HB3	1:B:480:THR:CG2	2.38	0.53
1:B:1973:ARG:HA	1:B:1976:ASP:HB2	1.91	0.53
1:B:1141:LYS:HG3	1:B:1145:LYS:HE3	1.89	0.53
1:B:1499:ASP:OD2	1:B:1763:ARG:NH1	2.35	0.53
1:B:1693:ARG:HD3	1:B:1697:ASP:OD2	2.08	0.53
2:J:2135:ASP:N	2:J:2135:ASP:OD1	2.41	0.53
1:B:988:ALA:HB2	1:B:998:VAL:HG11	1.91	0.52
1:B:1864:GLU:HA	1:B:1867:LEU:HD12	1.89	0.52
1:B:2017:ILE:HD13	1:B:2043:ARG:HB2	1.90	0.52
1:B:2013:ARG:NH1	1:B:2049:GLY:H	2.07	0.52
1:B:2043:ARG:HD2	1:B:2046:GLU:HB2	1.91	0.52
1:B:1140:VAL:HA	1:B:1143:ILE:HD12	1.91	0.52
1:B:630:ALA:HB2	1:B:900:MET:HE3	1.91	0.52
1:B:1307:LEU:HB2	1:B:1333:THR:HG23	1.91	0.52
1:B:1229:ASP:OD2	3:B:5803:QAU:O10	2.29	0.51
1:B:1764:MET:HE3	1:B:1773:LEU:HD11	1.92	0.51
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.46	0.51
1:B:757:ALA:O	1:B:761:VAL:HG23	2.11	0.51
1:B:2051:VAL:HG13	1:B:2113:TYR:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1547:TYR:O	1:B:1551:THR:HG23	2.11	0.51
1:B:1050:GLU:OE2	5:B:5904:HOH:O	2.19	0.50
1:B:1868:LEU:HD23	1:B:1871:LEU:HD12	1.94	0.50
1:B:700:ARG:HH21	1:B:872:SER:HB3	1.76	0.50
1:B:726:HIS:NE2	1:B:830:GLY:O	2.34	0.50
1:B:728:ARG:HH11	1:B:787:ALA:HB3	1.77	0.50
1:B:1905:SER:HB2	1:B:1908:LEU:HB2	1.92	0.50
1:B:517:MET:HE3	1:B:559:LEU:HD11	1.94	0.50
2:J:2089:HIS:NE2	5:J:2402:HOH:O	2.32	0.49
1:B:832:GLN:NE2	1:B:843:GLU:OE2	2.42	0.49
1:B:1661:VAL:O	1:B:1702:CYS:HA	2.11	0.49
1:B:544:MET:HE3	4:B:5808:EDO:H12	1.93	0.49
1:B:522:GLY:O	1:B:525:ILE:HG22	2.13	0.49
1:B:1864:GLU:O	1:B:1867:LEU:HB2	2.13	0.48
1:B:438:GLN:NE2	1:B:439:ARG:O	2.44	0.48
1:B:1158:HIS:HA	1:B:1161:ILE:HG22	1.95	0.48
1:B:575:LEU:HD11	1:B:1240:LEU:HD11	1.96	0.48
1:B:973:ASP:O	1:B:977:GLY:N	2.46	0.48
1:B:1211:ASP:OD1	1:B:1213:LYS:HG2	2.14	0.48
1:B:2029:ILE:HG23	1:B:2126:VAL:HA	1.94	0.48
1:B:1192:PRO:HG3	1:B:1289:LEU:HD11	1.94	0.48
1:B:1905:SER:HB3	1:B:1908:LEU:HD13	1.95	0.47
1:B:545:ARG:HG3	4:B:5807:EDO:H11	1.96	0.47
1:B:557:LYS:HE2	1:B:557:LYS:HB2	1.66	0.47
1:B:815:LEU:HD11	1:B:821:LEU:HD23	1.97	0.47
1:B:1886:ASP:O	1:B:1889:VAL:HG22	2.14	0.47
1:B:514:LEU:HD12	1:B:517:MET:CE	2.45	0.47
1:B:1601:LEU:O	1:B:1610:LYS:HD3	2.15	0.47
1:B:1900:SER:HB2	1:B:1954:TRP:NE1	2.24	0.47
2:J:2059:PRO:HG2	2:J:2063:MET:HB2	1.96	0.47
2:J:2090:ILE:HG21	2:J:2111:LEU:HD21	1.96	0.47
1:B:1456:VAL:HG12	1:B:1491:SER:HB2	1.96	0.47
1:B:1328:PHE:HB3	1:B:1332:GLN:HB2	1.97	0.47
1:B:1585:GLN:CB	1:B:1588:ARG:HD2	2.44	0.47
1:B:1648:ARG:HG3	1:B:1649:SER:N	2.30	0.47
1:B:1031:GLU:HA	1:B:1034:LYS:HD2	1.97	0.46
1:B:1269:ARG:HD2	1:B:1279:GLU:OE2	2.14	0.46
2:J:2058:GLY:HA2	2:J:2059:PRO:HD3	1.67	0.46
1:B:699:LYS:O	1:B:703:ILE:HG13	2.15	0.46
1:B:690:VAL:HG11	1:B:707:ILE:HD13	1.96	0.46
1:B:1195:ARG:HD3	1:B:1260:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:PRO:HG3	1:B:893:MET:HA	1.97	0.46
1:B:968:ASN:ND2	5:B:5923:HOH:O	2.48	0.46
1:B:1515:HIS:CD2	1:B:1721:PRO:HG3	2.50	0.46
1:B:1195:ARG:HG3	4:B:5809:EDO:H12	1.97	0.46
1:B:444:GLU:HG2	1:B:690:VAL:HG22	1.97	0.45
1:B:566:VAL:HG13	1:B:585:ILE:HB	1.98	0.45
1:B:1905:SER:CB	1:B:1908:LEU:HB2	2.47	0.45
2:J:2101:GLY:O	2:J:2138:GLN:NE2	2.49	0.45
2:J:2136:ASN:HD22	2:J:2136:ASN:H	1.63	0.45
1:B:544:MET:HG3	1:B:817:TRP:CD2	2.51	0.45
1:B:971:LYS:HB2	1:B:980:GLN:HB3	1.98	0.45
1:B:1577:LEU:HD11	1:B:1612:THR:HA	1.98	0.45
1:B:1840:THR:OG1	1:B:1938:PRO:HB3	2.17	0.45
1:B:1948:MET:HE3	1:B:1954:TRP:HA	1.98	0.45
1:B:403:LEU:O	1:B:406:ARG:NE	2.49	0.45
1:B:828:ILE:HD11	1:B:853:LEU:HG	1.97	0.45
1:B:1103:GLY:HA2	1:B:1233:ILE:HB	1.98	0.45
1:B:1262:LEU:HD21	1:B:1291:LEU:HD11	1.98	0.45
1:B:2042:GLU:HB3	1:B:2087:LYS:HZ2	1.82	0.45
1:B:514:LEU:HA	1:B:517:MET:HE2	1.99	0.45
1:B:1894:LEU:HD13	1:B:1912:THR:HG23	1.99	0.45
1:B:2026:LYS:HA	1:B:2026:LYS:HD3	1.73	0.45
1:B:760:GLU:O	1:B:764:THR:HG22	2.17	0.45
1:B:1876:PRO:HB2	1:B:1877:HIS:HD2	1.82	0.45
1:B:1879:LEU:HG	1:B:1880:ASN:H	1.82	0.45
1:B:1357:THR:O	1:B:1361:GLU:HG3	2.17	0.45
2:J:2252:LEU:HB2	2:J:2255:HIS:CE1	2.52	0.44
1:B:1456:VAL:HG12	1:B:1490:LEU:O	2.18	0.44
1:B:967:ASN:OD1	1:B:999:GLN:HG3	2.18	0.44
1:B:1335:VAL:O	1:B:1339:VAL:HG23	2.18	0.44
1:B:1822:TYR:O	1:B:1921:ARG:HD2	2.17	0.44
1:B:1837:ASN:C	1:B:1839:LYS:H	2.26	0.44
1:B:893:MET:HE3	1:B:900:MET:SD	2.57	0.44
1:B:1584:ILE:H	1:B:1584:ILE:HG13	1.44	0.44
1:B:1660:LEU:HA	1:B:1701:ARG:O	2.18	0.44
1:B:2077:ILE:HG23	1:B:2094:PHE:CD1	2.52	0.44
1:B:2059:LYS:HD2	1:B:2059:LYS:N	2.33	0.44
1:B:2099:THR:HA	1:B:2126:VAL:HB	1.99	0.44
1:B:1892:ASN:O	1:B:1896:GLN:HG2	2.17	0.44
1:B:1900:SER:N	1:B:1954:TRP:HE1	2.15	0.44
2:J:2059:PRO:HB3	2:J:2062:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1136:PRO:O	1:B:1139:VAL:HG22	2.18	0.43
1:B:1223:ILE:O	1:B:1236:HIS:HA	2.17	0.43
1:B:1753:ASP:O	1:B:1756:THR:HB	2.18	0.43
1:B:1732:MET:HB3	1:B:1732:MET:HE2	1.61	0.43
1:B:403:LEU:HA	1:B:954:LEU:HD21	2.00	0.43
1:B:455:PHE:HD2	1:B:459:GLU:HG3	1.84	0.43
1:B:2029:ILE:HG12	1:B:2030:ARG:N	2.33	0.43
1:B:1130:ARG:NH2	1:B:1144:GLU:OE2	2.45	0.43
1:B:2019:LEU:HD11	1:B:2039:VAL:HG13	2.01	0.43
1:B:1625:SER:HB3	1:B:1628:GLU:HG3	2.01	0.43
1:B:1862:HIS:O	1:B:1865:ASP:HB2	2.19	0.43
1:B:1731:CYS:HB2	5:B:6103:HOH:O	2.18	0.43
1:B:1586:ARG:HD2	1:B:1587:GLN:N	2.33	0.43
2:J:2076:ARG:HB3	2:J:2305:TYR:OH	2.18	0.43
2:J:2147:MET:O	2:J:2274:PRO:HD3	2.19	0.43
1:B:1607:SER:O	1:B:1611:GLU:HG3	2.19	0.42
1:B:1930:LEU:HD13	1:B:1938:PRO:C	2.44	0.42
1:B:1936:LEU:HD11	1:B:2107:TYR:HE2	1.83	0.42
1:B:542:ALA:O	1:B:589:THR:HA	2.19	0.42
1:B:1577:LEU:HD23	1:B:1577:LEU:HA	1.83	0.42
1:B:638:ASN:HA	1:B:641:MET:HG2	2.01	0.42
1:B:1211:ASP:HB3	1:B:1214:VAL:HG12	2.02	0.42
1:B:1351:PRO:O	1:B:1354:SER:OG	2.23	0.42
1:B:2042:GLU:HB3	1:B:2087:LYS:NZ	2.34	0.42
1:B:1864:GLU:O	1:B:1868:LEU:HG	2.19	0.42
1:B:1897:ALA:HA	1:B:1902:MET:HG2	2.02	0.42
1:B:2047:VAL:HG21	1:B:2085:GLN:HA	2.02	0.42
1:B:436:ARG:HE	1:B:443:GLU:CD	2.28	0.42
1:B:944:LYS:HE2	1:B:944:LYS:HB3	1.92	0.42
1:B:1598:ILE:N	1:B:1599:PRO:HD2	2.35	0.42
1:B:1763:ARG:HD2	1:B:1763:ARG:HA	1.84	0.42
1:B:1914:GLU:O	1:B:1917:SER:OG	2.29	0.42
1:B:1368:LEU:HD22	1:B:1403:LYS:HE3	2.02	0.42
1:B:2068:ILE:HG13	1:B:2092:LEU:HD12	2.02	0.42
1:B:571:GLY:HA2	1:B:592:LYS:NZ	2.35	0.42
1:B:966:LYS:HE3	5:B:6204:HOH:O	2.20	0.42
1:B:543:PRO:HD2	1:B:547:LEU:HD23	2.02	0.41
1:B:1172:LYS:HB2	1:B:1172:LYS:HE3	1.81	0.41
1:B:1195:ARG:HH11	1:B:1260:GLU:CD	2.27	0.41
1:B:1138:GLU:H	1:B:1138:GLU:CD	2.28	0.41
1:B:1608:THR:O	1:B:1612:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:ILE:HD13	1:B:721:VAL:HG21	2.03	0.41
1:B:822:PRO:HG2	1:B:858:ARG:HG2	2.02	0.41
1:B:2019:LEU:HD13	1:B:2041:LEU:HD23	2.01	0.41
1:B:935:LEU:HD23	1:B:935:LEU:HA	1.80	0.41
1:B:1071:LYS:HD2	1:B:1071:LYS:HA	1.76	0.41
1:B:1735:HIS:O	1:B:1739:GLU:HG2	2.20	0.41
1:B:2019:LEU:HD23	1:B:2120:TYR:CE2	2.55	0.41
1:B:493:LEU:O	1:B:519:ARG:HD2	2.20	0.41
1:B:580:ILE:HD12	1:B:580:ILE:H	1.85	0.41
1:B:721:VAL:HG13	1:B:808:VAL:HG22	2.02	0.41
1:B:827:ILE:HG12	1:B:868:ILE:HD12	2.02	0.41
1:B:1824:ILE:HD13	1:B:1922:LEU:HD23	2.03	0.41
1:B:1909:GLN:O	1:B:1912:THR:OG1	2.33	0.41
1:B:1224:LEU:HD23	1:B:1236:HIS:HB2	2.02	0.41
1:B:1620:LEU:HD12	1:B:1654:MET:HE3	2.03	0.41
1:B:1141:LYS:HA	1:B:1141:LYS:HD2	1.92	0.40
1:B:1808:MET:HG3	1:B:1809:ASP:OD1	2.21	0.40
1:B:1435:LEU:HD23	1:B:1435:LEU:HA	1.81	0.40
1:B:1869:ARG:HD2	1:B:1869:ARG:HA	1.87	0.40
1:B:1934:GLY:HA2	1:B:2076:LEU:HB3	2.03	0.40
1:B:1960:LEU:HD11	1:B:1980:GLU:HA	2.03	0.40
2:J:2100:THR:O	2:J:2259:VAL:HG12	2.21	0.40
1:B:1939:ALA:O	1:B:1943:MET:HG3	2.21	0.40
2:J:2113:LYS:O	2:J:2117:ILE:HG23	2.22	0.40
1:B:608:LEU:O	1:B:610:ARG:HG2	2.21	0.40
1:B:760:GLU:HG3	1:B:763:ARG:NH1	2.25	0.40
1:B:760:GLU:OE1	1:B:760:GLU:N	2.53	0.40
2:J:2154:HIS:CD2	2:J:2155:GLN:HG2	2.56	0.40
1:B:733:LYS:HD3	1:B:736:ARG:HH21	1.86	0.40
1:B:1515:HIS:CE1	1:B:1721:PRO:HG3	2.56	0.40
1:B:1633:GLU:HG2	1:B:1656:VAL:HG13	2.03	0.40
1:B:2094:PHE:CZ	1:B:2097:PRO:HD3	2.57	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	1724/1747 (99%)	1672 (97%)	48 (3%)	4 (0%)	43	52
2	J	261/263 (99%)	254 (97%)	6 (2%)	1 (0%)	30	34
All	All	1985/2010 (99%)	1926 (97%)	54 (3%)	5 (0%)	36	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	533	VAL
1	B	1901	ARG
1	B	2045	GLU
2	J	2059	PRO
1	B	2097	PRO

### 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	1545/1560 (99%)	1482 (96%)	63 (4%)	27	36
2	J	236/236 (100%)	230 (98%)	6 (2%)	42	55
All	All	1781/1796 (99%)	1712 (96%)	69 (4%)	28	39

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	510	THR
1	B	541	ILE
1	B	572	ASP
1	B	579	GLU
1	B	585	ILE
1	B	604	THR
1	B	683	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	721	VAL
1	B	758	SER
1	B	819	VAL
1	B	837	GLU
1	B	893	MET
1	B	935	LEU
1	B	966	LYS
1	B	984	LEU
1	B	992	TYR
1	B	1008	THR
1	B	1032	GLU
1	B	1044	VAL
1	B	1051	SER
1	B	1071	LYS
1	B	1086	GLN
1	B	1126	MET
1	B	1157	ASN
1	B	1172	LYS
1	B	1271	VAL
1	B	1313	ARG
1	B	1342	SER
1	B	1358	ILE
1	B	1371	SER
1	B	1373	GLU
1	B	1387	GLU
1	B	1434	ILE
1	B	1511	THR
1	B	1523	LEU
1	B	1536	GLN
1	B	1551	THR
1	B	1584	ILE
1	B	1605	SER
1	B	1622	GLU
1	B	1630	ARG
1	B	1787	GLU
1	B	1842	VAL
1	B	1856	GLU
1	B	1883	LYS
1	B	1905	SER
1	B	1907	GLU
1	B	1937	SER
1	B	1944	GLU

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Mol	Chain	Res	Type
1	B	1945	LEU
1	B	1948	MET
1	B	1985	ILE
1	B	1991	GLU
1	B	1999	LEU
1	B	2017	ILE
1	B	2026	LYS
1	B	2029	ILE
1	B	2031	SER
1	B	2076	LEU
1	B	2082	LEU
1	B	2083	THR
1	B	2084	LEU
1	B	2116	CYS
2	J	2093	SER
2	J	2100	THR
2	J	2135	ASP
2	J	2136	ASN
2	J	2233	SER
2	J	2239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	705	ASN
1	B	715	HIS
1	B	771	ASN
1	B	877	GLN
1	B	1038	GLN
1	B	1069	GLN
1	B	1157	ASN
1	B	1526	HIS
1	B	1692	ASN
1	B	1730	HIS
1	B	1791	GLN
1	B	1814	ASN
1	B	1885	ASN
1	B	1933	ASN
2	J	2089	HIS
2	J	2288	HIS
2	J	2291	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](#)

13 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
4	EDO	B	5804	-	3,3,3	0.29	0	2,2,2	1.06	0
4	EDO	B	5810	-	3,3,3	0.47	0	2,2,2	0.42	0
4	EDO	B	5808	-	3,3,3	0.45	0	2,2,2	0.32	0
3	QAU	B	5802	-	11,11,11	1.99	3 (27%)	15,16,16	3.75	5 (33%)
4	EDO	B	5812	-	3,3,3	0.48	0	2,2,2	0.46	0
4	EDO	B	5807	-	3,3,3	0.33	0	2,2,2	0.89	0
4	EDO	B	5809	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	B	5806	-	3,3,3	0.50	0	2,2,2	0.66	0
3	QAU	B	5801	-	11,11,11	2.02	2 (18%)	15,16,16	3.29	4 (26%)
4	EDO	B	5813	-	3,3,3	0.40	0	2,2,2	0.63	0
4	EDO	B	5811	-	3,3,3	0.41	0	2,2,2	0.72	0
4	EDO	B	5805	-	3,3,3	0.34	0	2,2,2	1.16	0
3	QAU	B	5803	-	11,11,11	2.35	3 (27%)	15,16,16	3.27	4 (26%)

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
4	EDO	B	5804	-	-	1/1/1/1	-
4	EDO	B	5810	-	-	0/1/1/1	-
4	EDO	B	5808	-	-	0/1/1/1	-
3	QAU	B	5802	-	-	2/6/6/6	0/1/1/1
4	EDO	B	5812	-	-	1/1/1/1	-
4	EDO	B	5807	-	-	1/1/1/1	-
4	EDO	B	5809	-	-	1/1/1/1	-
4	EDO	B	5806	-	-	1/1/1/1	-
3	QAU	B	5801	-	-	2/6/6/6	0/1/1/1
4	EDO	B	5813	-	-	1/1/1/1	-
4	EDO	B	5811	-	-	1/1/1/1	-
4	EDO	B	5805	-	-	1/1/1/1	-
3	QAU	B	5803	-	-	0/6/6/6	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5803	QAU	S02-N01	5.75	1.71	1.60
3	B	5801	QAU	S02-N01	5.48	1.71	1.60
3	B	5802	QAU	S02-N01	4.73	1.69	1.60
3	B	5803	QAU	C05-S02	3.89	1.83	1.77
3	B	5802	QAU	C05-S02	2.99	1.81	1.77
3	B	5801	QAU	C05-S02	2.66	1.81	1.77
3	B	5802	QAU	O03-S02	2.46	1.48	1.43
3	B	5803	QAU	O04-S02	2.30	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5802	QAU	O04-S02-O03	-11.66	100.86	118.80
3	B	5801	QAU	O04-S02-O03	-10.64	102.43	118.80
3	B	5803	QAU	O04-S02-O03	-10.54	102.59	118.80
3	B	5802	QAU	O03-S02-C05	5.44	113.50	107.35
3	B	5801	QAU	O03-S02-C05	4.93	112.92	107.35
3	B	5802	QAU	O04-S02-N01	4.70	114.13	107.35
3	B	5803	QAU	O03-S02-C05	4.57	112.52	107.35
3	B	5801	QAU	O04-S02-N01	3.67	112.64	107.35
3	B	5803	QAU	O04-S02-N01	3.37	112.22	107.35
3	B	5802	QAU	O04-S02-C05	2.91	110.64	107.35
3	B	5803	QAU	O04-S02-C05	2.91	110.64	107.35
3	B	5802	QAU	O03-S02-N01	2.71	111.25	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5801	QAU	O03-S02-N01	2.02	110.27	107.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

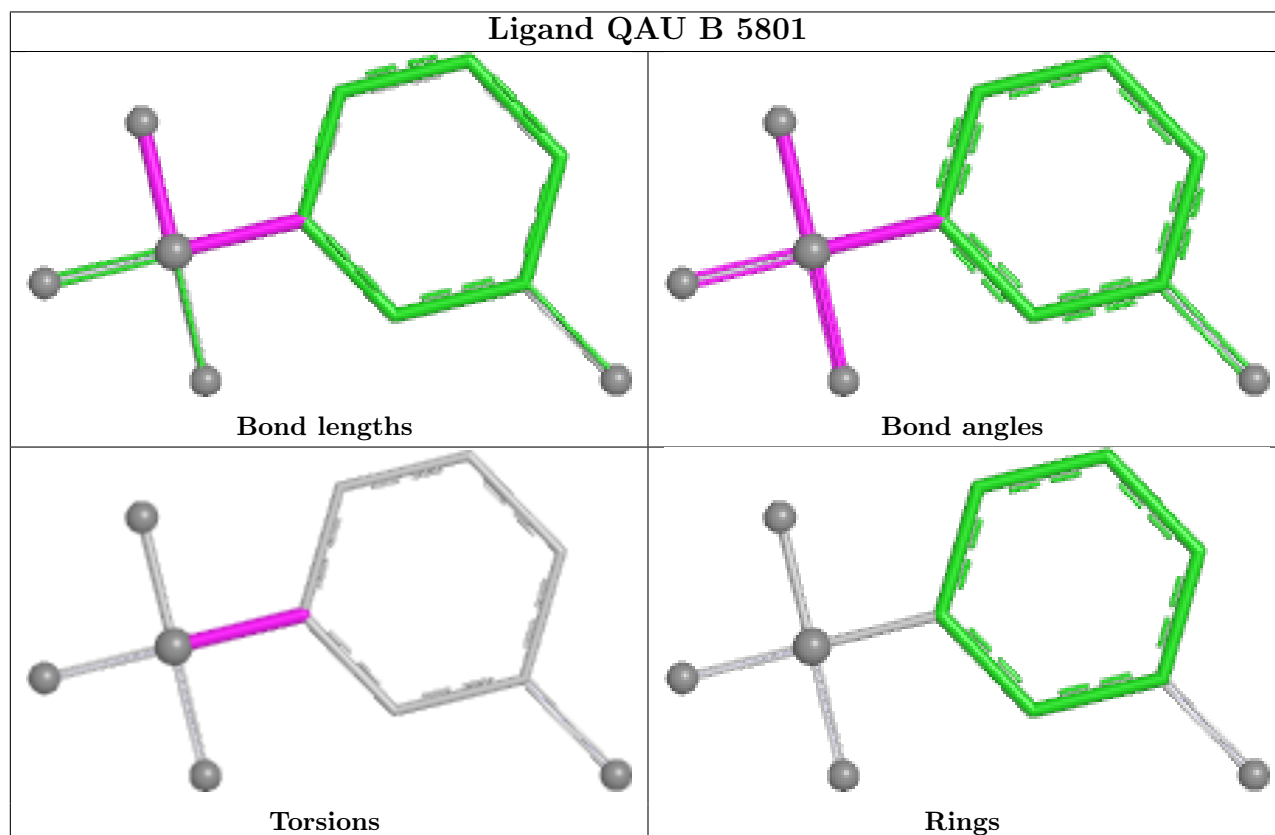
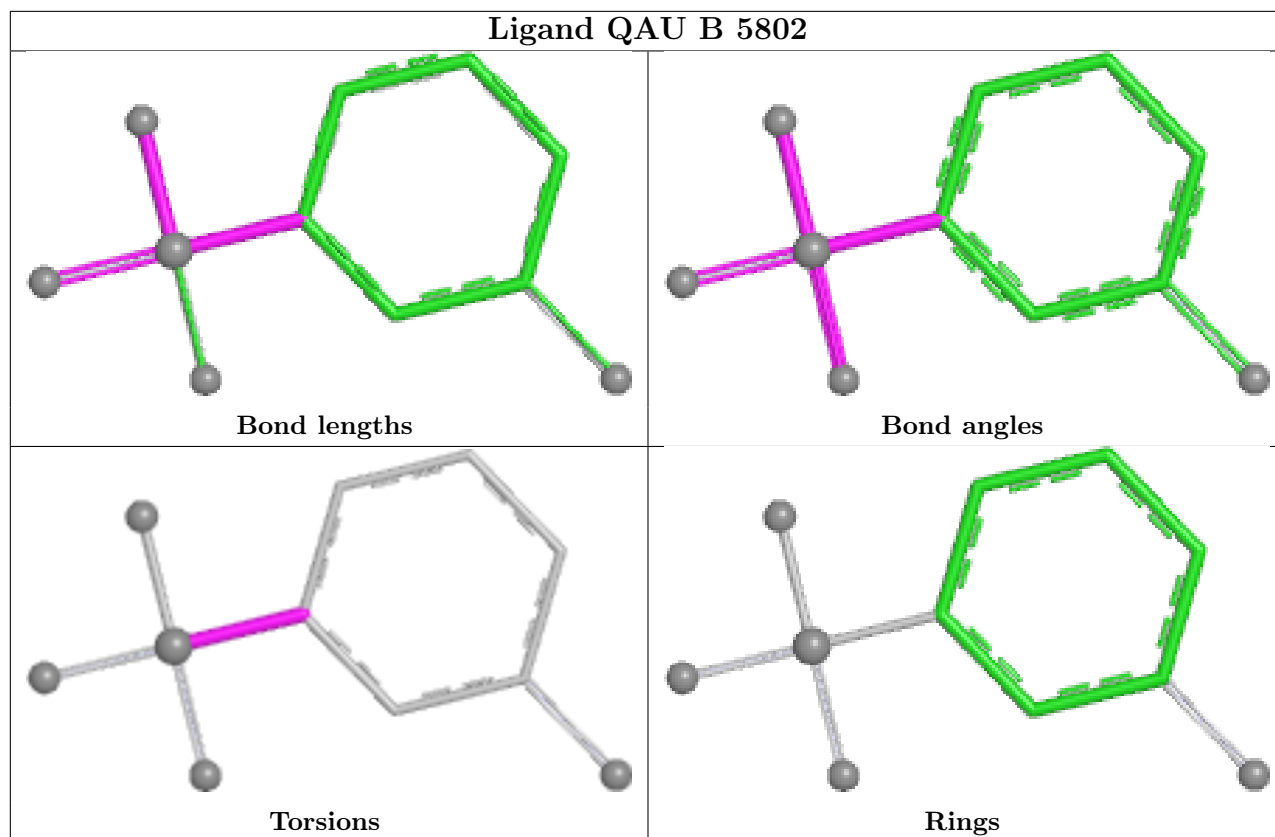
Mol	Chain	Res	Type	Atoms
4	B	5809	EDO	O1-C1-C2-O2
3	B	5801	QAU	C11-C05-S02-O04
4	B	5805	EDO	O1-C1-C2-O2
3	B	5801	QAU	C06-C05-S02-O04
3	B	5802	QAU	C11-C05-S02-O03
4	B	5811	EDO	O1-C1-C2-O2
4	B	5813	EDO	O1-C1-C2-O2
3	B	5802	QAU	C06-C05-S02-O03
4	B	5812	EDO	O1-C1-C2-O2
4	B	5804	EDO	O1-C1-C2-O2
4	B	5806	EDO	O1-C1-C2-O2
4	B	5807	EDO	O1-C1-C2-O2

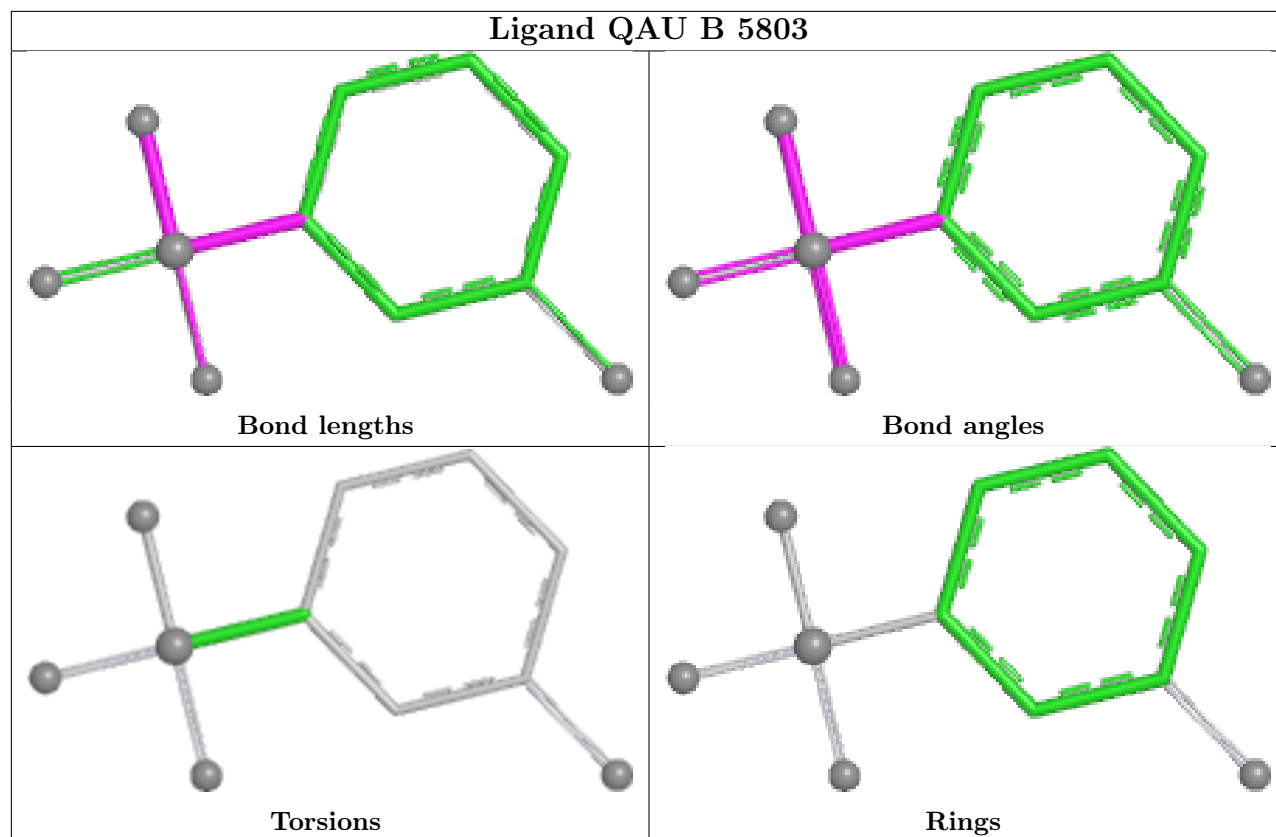
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5808	EDO	1	0
4	B	5807	EDO	1	0
4	B	5809	EDO	2	0
3	B	5803	QAU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1725/1747 (98%)	0.45	109 (6%) 26 29	29, 58, 128, 177	1 (0%)
2	J	263/263 (100%)	0.22	12 (4%) 37 43	34, 54, 111, 197	0
All	All	1988/2010 (98%)	0.42	121 (6%) 27 31	29, 57, 128, 197	1 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	403	LEU	6.1
1	B	1996	LEU	6.1
1	B	1584	ILE	5.6
1	B	1601	LEU	5.4
1	B	404	ALA	5.1
2	J	2058	GLY	4.8
1	B	1904	LEU	4.1
1	B	576	CYS	4.0
2	J	2060	LEU	3.9
1	B	2038	LEU	3.9
1	B	1875	VAL	3.8
1	B	570	THR	3.7
2	J	2097	ILE	3.6
2	J	2318	ALA	3.5
1	B	2124	VAL	3.4
1	B	455	PHE	3.4
1	B	1884	PHE	3.4
1	B	1903	GLN	3.3
1	B	1899	LEU	3.3
1	B	1515	HIS	3.3
1	B	575	LEU	3.3
1	B	1936	LEU	3.3
1	B	1902	MET	3.2
1	B	1840	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1849	ILE	3.2
1	B	600	GLY	3.2
1	B	574	GLN	3.1
1	B	1136	PRO	3.1
1	B	582	ALA	3.0
1	B	2112	ALA	3.0
1	B	1908	LEU	3.0
1	B	2024	VAL	3.0
1	B	1867	LEU	3.0
1	B	1960	LEU	3.0
1	B	1999	LEU	3.0
1	B	573	HIS	3.0
1	B	1998	GLN	3.0
1	B	1845	LEU	3.0
1	B	1893	LEU	2.9
1	B	2041	LEU	2.9
1	B	726	HIS	2.9
1	B	701	PHE	2.9
1	B	1871	LEU	2.9
1	B	1879	LEU	2.9
1	B	1997	LEU	2.9
1	B	2036	VAL	2.9
1	B	405	PRO	2.8
2	J	2063	MET	2.8
1	B	1161	ILE	2.8
1	B	454	PRO	2.8
1	B	1995	ALA	2.8
1	B	1151	GLU	2.8
1	B	580	ILE	2.8
1	B	1598	ILE	2.8
2	J	2319	LEU	2.8
1	B	1842	VAL	2.8
1	B	1954	TRP	2.8
1	B	2068	ILE	2.8
1	B	1979	VAL	2.8
1	B	1074	GLY	2.7
1	B	2034	PRO	2.7
1	B	2098	ALA	2.7
1	B	1328	PHE	2.6
1	B	1593	THR	2.6
1	B	601	GLY	2.6
1	B	1140	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	2097	PRO	2.6
1	B	1868	LEU	2.5
1	B	1872	ALA	2.5
1	B	1165	ILE	2.5
1	B	1863	HIS	2.5
1	B	2052	ILE	2.5
1	B	1963	LEU	2.5
2	J	2098	LYS	2.5
1	B	2023	VAL	2.5
1	B	1901	ARG	2.5
1	B	1966	PHE	2.5
1	B	2126	VAL	2.4
1	B	755	GLY	2.4
1	B	1865	ASP	2.4
1	B	1906	ALA	2.4
1	B	1139	VAL	2.4
1	B	1971	ILE	2.4
1	B	1604	LEU	2.4
1	B	603	ARG	2.4
1	B	2005	ALA	2.3
1	B	2047	VAL	2.3
1	B	1940	LEU	2.3
1	B	2004	ILE	2.3
2	J	2062	SER	2.3
1	B	1846	ILE	2.3
1	B	1889	VAL	2.3
2	J	2286	VAL	2.2
1	B	1882	PRO	2.2
1	B	2071	ALA	2.2
1	B	1895	LEU	2.2
1	B	1974	CYS	2.2
1	B	2000	THR	2.2
1	B	2002	SER	2.2
1	B	1985	ILE	2.2
1	B	1876	PRO	2.2
2	J	2071	THR	2.2
1	B	525	ILE	2.1
1	B	1170	MET	2.1
1	B	1075	PHE	2.1
1	B	456	GLY	2.1
1	B	604	THR	2.1
1	B	1321	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1603	LYS	2.1
2	J	2247	ASN	2.1
1	B	1585	GLN	2.1
1	B	571	GLY	2.1
1	B	1135	LEU	2.1
1	B	642	THR	2.1
1	B	2008	ALA	2.1
1	B	1843	ARG	2.1
1	B	754	GLU	2.0
1	B	1836	LEU	2.0
1	B	1866	ASN	2.0
1	B	792	VAL	2.0
2	J	2093	SER	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.

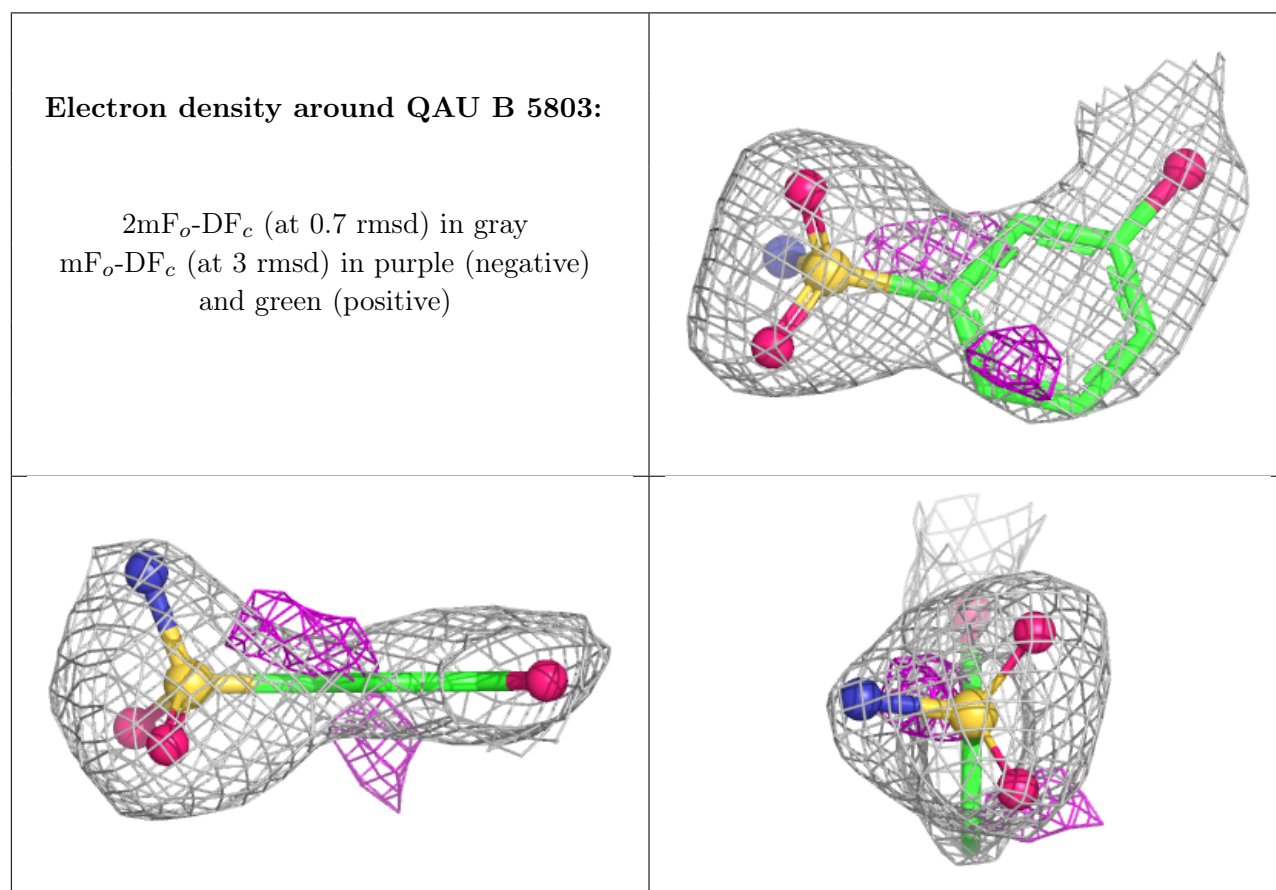
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	5813	4/4	0.76	0.21	72,73,78,84	0
4	EDO	B	5808	4/4	0.77	0.14	57,59,62,64	0
4	EDO	B	5812	4/4	0.79	0.18	69,76,76,79	0
4	EDO	B	5810	4/4	0.81	0.14	52,54,57,63	0
4	EDO	B	5809	4/4	0.85	0.15	46,50,50,50	0
4	EDO	B	5811	4/4	0.87	0.10	52,53,59,61	0
4	EDO	B	5805	4/4	0.90	0.11	45,46,47,48	0
4	EDO	B	5806	4/4	0.91	0.11	37,39,40,41	0
4	EDO	B	5807	4/4	0.91	0.11	47,47,48,52	0
3	QAU	B	5803	11/11	0.94	0.09	45,50,53,57	0

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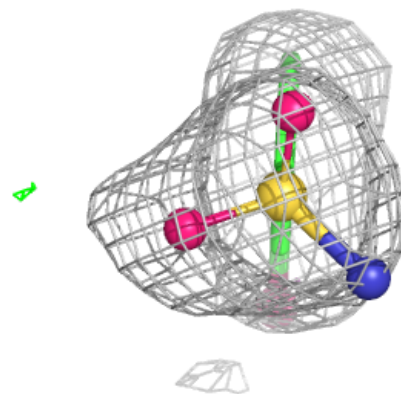
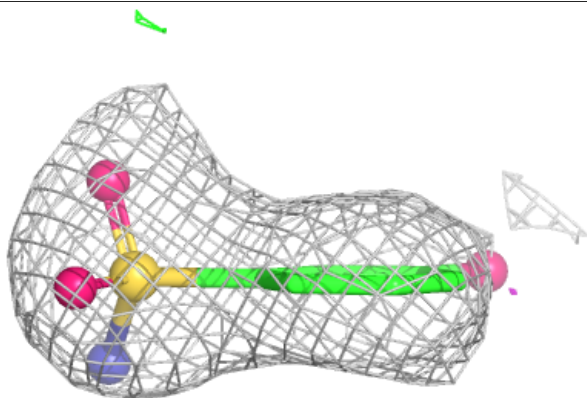
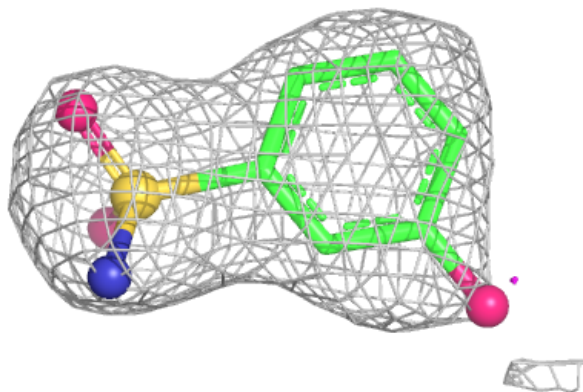
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	5804	4/4	0.95	0.08	39,41,44,45	0
3	QAU	B	5801	11/11	0.95	0.10	43,49,58,67	0
3	QAU	B	5802	11/11	0.96	0.07	40,44,46,48	0

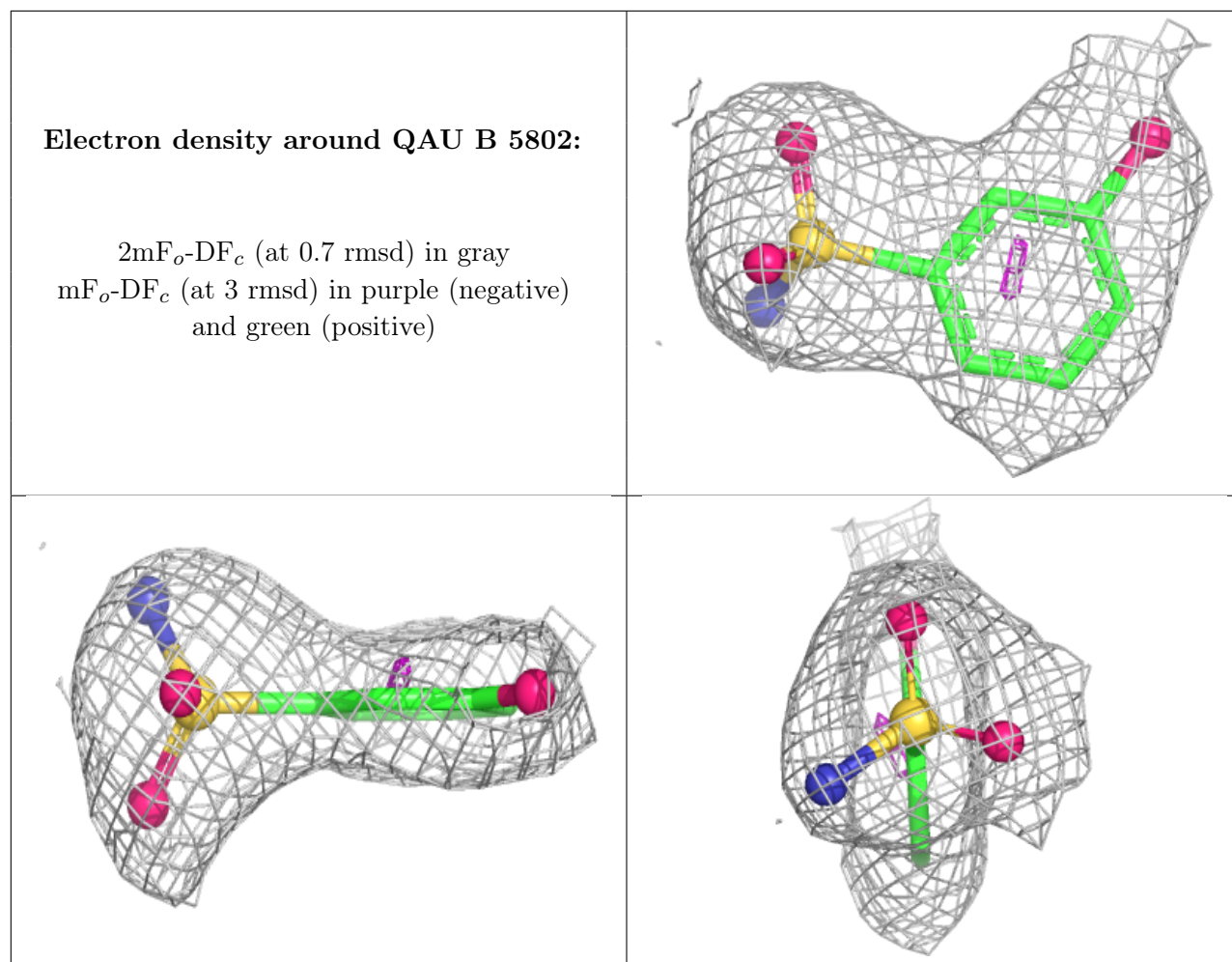
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around QAU B 5801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.