



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:03 PM UTC

PDB ID : 8BCA / pdb\_00008bca  
Title : Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and compound 26  
Authors : Vester, K.; Loll, B.; Wahl, M.C.  
Deposited on : 2022-10-15  
Resolution : 2.80 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

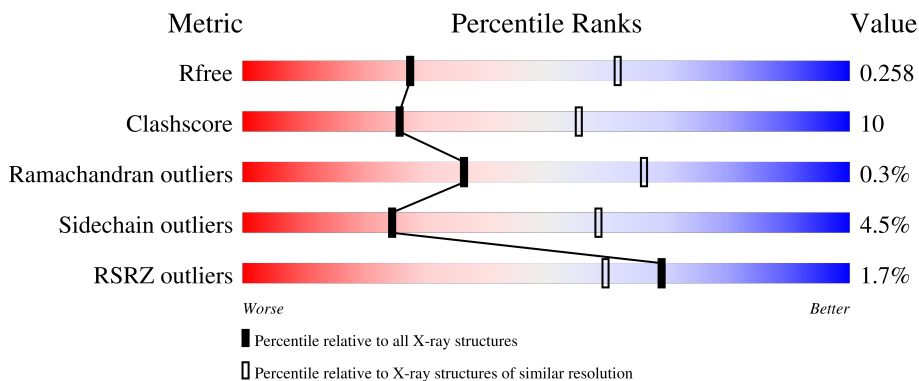
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	Q96	B	5802	-	X	-	-
4	EDO	B	5806	-	-	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 16236 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	1724	13870	8864	2372	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

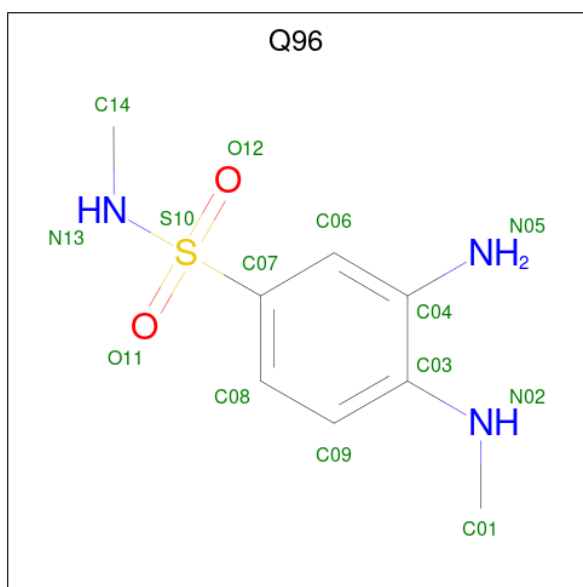
- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

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-azanyl- {N}-methyl-4-(methylamino)benzenesulfonamide (CCD ID: Q96) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>3</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
3	B	1	Total	14	8	3	2	1	0	0
3	B	1	Total	14	8	3	2	1	0	0

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



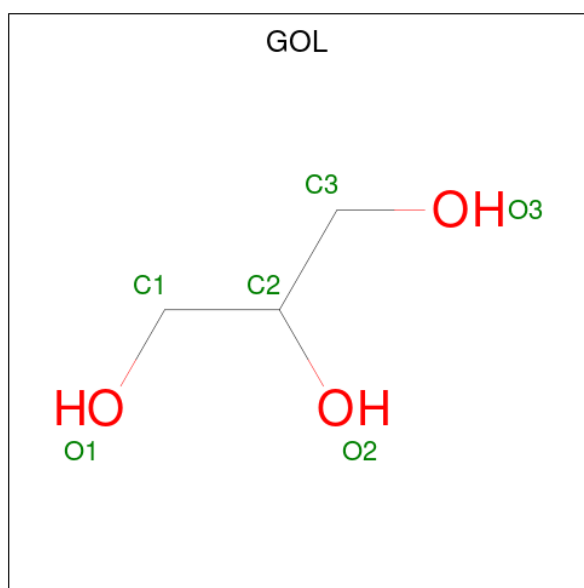
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			
4	B	1	Total	4	2	2	0	0
4	B	1	Total	4	2	2	0	0

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	155	Total	O	0	0
			155	155		

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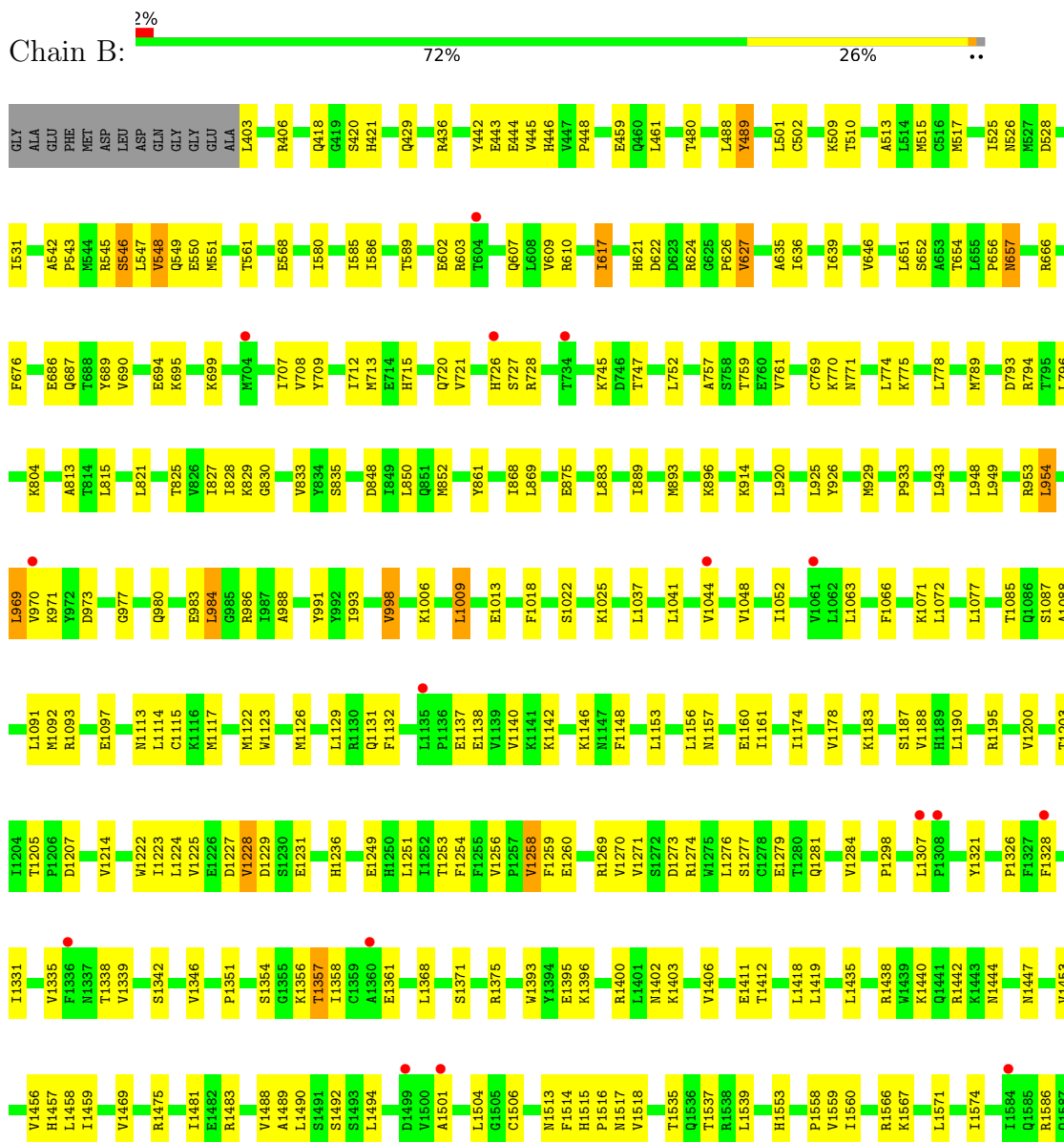
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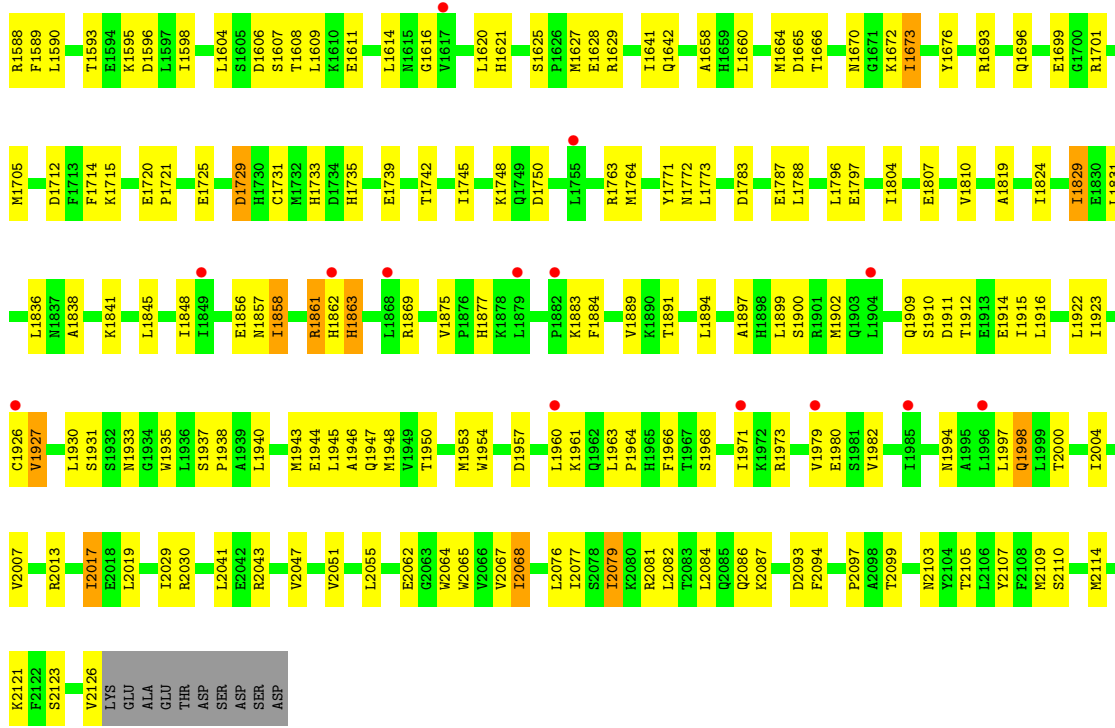
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	J	18	Total	O	0	0
			18	18		

### 3 Residue-property plots i

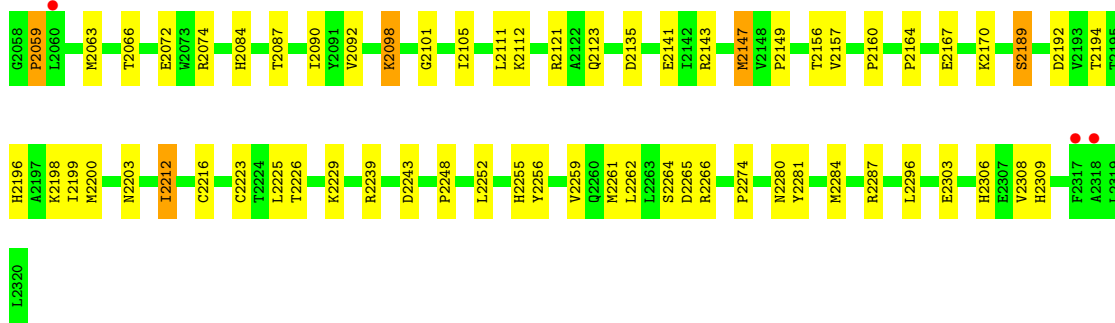
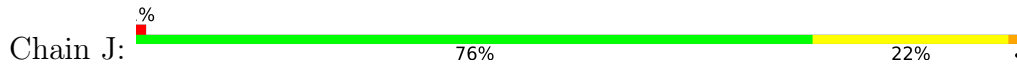
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, $\alpha$ , $\beta$ , $\gamma$	100.41Å 119.36Å 187.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 2.80 48.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.53-2.80) 99.5 (48.53-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, $R_{free}$	0.199 , 0.258 0.200 , 0.258	Depositor DCC
$R_{free}$ test set	2100 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.5	Xtrriage
Anisotropy	0.129	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 34.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: EDO, GOL, Q96

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B	0.26	0/14164	0.45	0/19192
2	J	0.26	0/2190	0.46	0/2981
All	All	0.26	0/16354	0.45	0/22173

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	13870	0	14008	274	1
2	J	2123	0	2063	34	0
3	B	28	0	0	0	0
4	B	36	0	53	6	0
5	B	6	0	8	0	0
6	B	155	0	0	7	0
6	J	18	0	0	0	0
All	All	16236	0	16132	307	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 10.

All (307) 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:1227:ASP:HB2	4:B:5806:EDO:H11	1.55	0.88
1:B:1558:PRO:HD2	1:B:1693:ARG:HH12	1.42	0.82
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	1.63	0.81
1:B:1229:ASP:HB2	1:B:1231:GLU:HG2	1.65	0.78
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.65	0.77
1:B:1481:ILE:HG22	1:B:1483:ARG:H	1.51	0.76
1:B:1586:ARG:HH12	1:B:1588:ARG:HD3	1.48	0.76
1:B:1894:LEU:HB3	1:B:1912:THR:HG22	1.68	0.75
1:B:525:ILE:HG12	1:B:531:ILE:HG13	1.69	0.74
1:B:436:ARG:HG2	1:B:445:VAL:HG22	1.73	0.71
2:J:2087:THR:HB	2:J:2112:LYS:HD3	1.72	0.71
1:B:2019:LEU:HB3	1:B:2041:LEU:HD23	1.71	0.71
2:J:2141:GLU:OE1	2:J:2143:ARG:NH2	2.23	0.71
2:J:2164:PRO:HB3	2:J:2296:LEU:HD11	1.73	0.69
1:B:1869:ARG:HD3	1:B:1884:PHE:HZ	1.57	0.69
1:B:1298:PRO:HB3	1:B:1515:HIS:CG	2.27	0.69
1:B:1259:PHE:HE2	4:B:5806:EDO:H22	1.58	0.69
1:B:1672:LYS:NZ	1:B:1856:GLU:OE1	2.24	0.69
1:B:1862:HIS:CG	1:B:1863:HIS:H	2.11	0.68
1:B:617:ILE:HG22	1:B:652:SER:HB2	1.75	0.68
1:B:687:GLN:OE1	1:B:689:TYR:OH	2.09	0.68
1:B:1406:VAL:HB	1:B:1418:LEU:HD22	1.75	0.68
1:B:420:SER:HB3	1:B:622:ASP:HA	1.75	0.68
1:B:1072:LEU:HD13	1:B:1077:LEU:HB3	1.76	0.68
1:B:993:ILE:HD12	1:B:1091:LEU:HD23	1.76	0.67
1:B:1361:GLU:OE2	1:B:1393:TRP:NE1	2.26	0.67
1:B:2017:ILE:HD11	1:B:2041:LEU:HB3	1.75	0.67
1:B:406:ARG:HD3	1:B:954:LEU:HD22	1.76	0.67
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	1.75	0.66
1:B:1944:GLU:HA	1:B:1947:GLN:HE21	1.60	0.66
1:B:546:SER:OG	6:B:5901:HOH:O	2.15	0.64
1:B:1900:SER:OG	1:B:1954:TRP:NE1	2.26	0.64
1:B:421:HIS:ND1	6:B:5902:HOH:O	2.30	0.63
1:B:848:ASP:HB3	1:B:852:MET:HE3	1.80	0.63
1:B:444:GLU:HG2	1:B:690:VAL:HG22	1.80	0.63
1:B:1501:ALA:HB1	1:B:1506:CYS:HB2	1.79	0.63
1:B:1607:SER:O	1:B:1611:GLU:HG2	1.98	0.63
1:B:1764:MET:HE3	1:B:1773:LEU:HD11	1.80	0.63
1:B:1269:ARG:HG2	1:B:1281:GLN:HG3	1.80	0.63
1:B:1586:ARG:NH1	1:B:1588:ARG:HD3	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1670:ASN:HB3	1:B:1673:ILE:HD11	1.80	0.63
2:J:2105:ILE:HD13	2:J:2262:LEU:HB2	1.81	0.63
1:B:971:LYS:HB2	1:B:980:GLN:HB3	1.81	0.63
1:B:1883:LYS:HB2	1:B:1889:VAL:HG21	1.80	0.62
1:B:624:ARG:O	1:B:627:VAL:HG13	1.99	0.62
1:B:1819:ALA:HB2	1:B:1829:ILE:HG21	1.82	0.62
1:B:636:ILE:HD13	1:B:666:ARG:HD2	1.82	0.62
1:B:2043:ARG:HB3	1:B:2086:GLN:HA	1.81	0.62
2:J:2196:HIS:HD2	2:J:2200:MET:HE2	1.65	0.61
1:B:920:LEU:HD23	1:B:953:ARG:HG2	1.83	0.60
2:J:2141:GLU:OE2	2:J:2266:ARG:NH2	2.32	0.60
1:B:2029:ILE:HG13	1:B:2126:VAL:HA	1.83	0.60
1:B:690:VAL:HG11	1:B:707:ILE:HD13	1.84	0.60
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.40	0.60
1:B:2030:ARG:HA	1:B:2126:VAL:HG13	1.84	0.59
1:B:991:TYR:OH	1:B:1097:GLU:OE1	2.19	0.59
1:B:448:PRO:HA	1:B:686[A]:GLU:HG3	1.84	0.59
1:B:1729:ASP:OD1	1:B:1729:ASP:N	2.35	0.58
1:B:1195:ARG:NH1	1:B:1260:GLU:OE1	2.37	0.57
2:J:2059:PRO:HB2	2:J:2063:MET:HB2	1.85	0.57
1:B:1944:GLU:O	1:B:1947:GLN:HG2	2.05	0.57
1:B:639:ILE:HD11	1:B:646:VAL:HB	1.86	0.57
2:J:2284:MET:HB3	2:J:2287:ARG:HD3	1.85	0.57
1:B:1456:VAL:HG21	1:B:1489:ALA:HB1	1.86	0.57
1:B:789:MET:HE2	1:B:794:ARG:HG2	1.88	0.56
2:J:2252:LEU:HB2	2:J:2255:HIS:CE1	2.41	0.56
1:B:1620:LEU:HD22	1:B:1629:ARG:HG3	1.87	0.56
1:B:1156:LEU:HD13	1:B:1160:GLU:HG3	1.87	0.56
2:J:2212:ILE:HG22	2:J:2229:LYS:HB3	1.87	0.56
1:B:1435:LEU:O	1:B:1442:ARG:NH1	2.39	0.55
2:J:2196:HIS:CD2	2:J:2200:MET:HE2	2.42	0.55
1:B:1515:HIS:CE1	1:B:1721:PRO:HG3	2.41	0.55
1:B:721:VAL:HG12	1:B:825:THR:HB	1.88	0.55
1:B:446:HIS:HB3	6:B:6008:HOH:O	2.07	0.55
1:B:1131:GLN:O	4:B:5812:EDO:H12	2.06	0.55
2:J:2212:ILE:HG21	2:J:2259:VAL:HG21	1.87	0.55
1:B:2051:VAL:HG22	1:B:2062:GLU:HG3	1.87	0.55
1:B:712:ILE:HG22	1:B:713:MET:HE2	1.87	0.55
1:B:1696:GLN:NE2	6:B:5903:HOH:O	2.36	0.54
1:B:1156:LEU:HD22	1:B:1160:GLU:HG2	1.88	0.54
1:B:545:ARG:NH2	1:B:549:GLN:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1122:MET:HE3	1:B:1126:MET:HB2	1.88	0.54
2:J:2194:THR:O	2:J:2198:LYS:HG2	2.07	0.54
1:B:2041:LEU:O	1:B:2087:LYS:HA	2.07	0.54
1:B:510:THR:HG21	1:B:551:MET:HE1	1.90	0.54
1:B:1037:LEU:HD13	1:B:1052:ILE:HD11	1.89	0.54
1:B:1269:ARG:NH1	1:B:1279:GLU:OE2	2.31	0.54
1:B:1438:ARG:HB2	1:B:1442:ARG:HD3	1.89	0.53
1:B:1588:ARG:HG3	1:B:1590:LEU:H	1.72	0.53
1:B:1909:GLN:O	1:B:1912:THR:OG1	2.20	0.53
1:B:1195:ARG:HD3	1:B:1260:GLU:OE2	2.09	0.53
1:B:1457:HIS:CE1	1:B:1492:SER:HB2	2.43	0.53
1:B:1456:VAL:O	1:B:1459:ILE:HG12	2.09	0.53
1:B:1307:LEU:HD23	1:B:1328:PHE:HD2	1.73	0.53
1:B:1396:LYS:O	1:B:1400:ARG:HB2	2.09	0.53
1:B:1973:ARG:HH12	1:B:1998:GLN:HB2	1.73	0.53
1:B:893:MET:HB3	1:B:925:LEU:HD22	1.91	0.52
1:B:1593:THR:HG22	1:B:1595:LYS:H	1.75	0.52
1:B:1660:LEU:HA	1:B:1701:ARG:O	2.10	0.52
1:B:1539:LEU:HD21	1:B:1665:ASP:HB2	1.92	0.52
2:J:2123:GLN:HB2	2:J:2157:VAL:HG22	1.90	0.52
1:B:1715:LYS:NZ	6:B:5905:HOH:O	2.42	0.52
2:J:2167:GLU:HG3	2:J:2170:LYS:NZ	2.25	0.52
2:J:2199:ILE:O	2:J:2203:ASN:ND2	2.34	0.52
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.45	0.52
1:B:1838:ALA:HA	1:B:1938:PRO:HG3	1.92	0.52
1:B:1475:ARG:HD2	1:B:1504:LEU:HA	1.91	0.52
1:B:1783:ASP:O	1:B:1787:GLU:HG3	2.11	0.51
1:B:815:LEU:HD11	1:B:821:LEU:HD23	1.90	0.51
1:B:828:ILE:HD12	1:B:869:LEU:HD12	1.92	0.51
1:B:436:ARG:HE	1:B:443:GLU:CD	2.19	0.51
1:B:1224:LEU:HD23	1:B:1236:HIS:HB2	1.92	0.51
1:B:1616:GLY:HA2	1:B:1641:ILE:HG22	1.92	0.51
1:B:421:HIS:NE2	1:B:875:GLU:OE1	2.32	0.51
2:J:2264:SER:OG	2:J:2265:ASP:N	2.43	0.51
2:J:2243:ASP:HB3	2:J:2248:PRO:HB3	1.91	0.51
1:B:689:TYR:HE2	1:B:883:LEU:HD12	1.75	0.50
1:B:1930:LEU:HD13	1:B:1938:PRO:HB2	1.92	0.50
1:B:1338:THR:O	1:B:1342:SER:HB2	2.11	0.50
1:B:1137:GLU:HA	1:B:1140:VAL:HG22	1.93	0.50
1:B:1946:ALA:O	1:B:1950:THR:HG23	2.12	0.50
1:B:656:PRO:O	1:B:657:ASN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1804:ILE:HG12	1:B:1810:VAL:HG12	1.92	0.50
1:B:969:LEU:HD21	1:B:998:VAL:HG23	1.93	0.50
1:B:1122:MET:HE2	1:B:1276:LEU:HD23	1.92	0.50
1:B:1943:MET:CE	1:B:2109:MET:HB2	2.41	0.50
1:B:774:LEU:HD22	1:B:778:LEU:HG	1.93	0.49
1:B:1604:LEU:HD23	1:B:1628:GLU:HG2	1.92	0.49
2:J:2149:PRO:HB3	2:J:2281:TYR:CE1	2.47	0.49
1:B:926:TYR:OH	1:B:948:LEU:O	2.27	0.49
1:B:1968:SER:HA	1:B:1971:ILE:HD12	1.93	0.49
1:B:1963:LEU:HD21	1:B:1982:VAL:HG13	1.93	0.49
1:B:770:LYS:HE2	1:B:796:LEU:HD22	1.94	0.49
1:B:1923:ILE:O	1:B:1927:VAL:HG13	2.12	0.49
1:B:1869:ARG:HD3	1:B:1884:PHE:CZ	2.42	0.49
2:J:2092:VAL:HG13	2:J:2261:MET:HE3	1.93	0.49
1:B:1438:ARG:HB2	1:B:1442:ARG:NH1	2.28	0.49
2:J:2072:GLU:OE1	2:J:2072:GLU:N	2.46	0.49
1:B:545:ARG:NH1	1:B:568:GLU:OE1	2.46	0.49
1:B:1725:GLU:OE1	1:B:1763:ARG:HD3	2.12	0.49
1:B:726:HIS:HB3	1:B:833:VAL:HG23	1.93	0.49
1:B:1346:VAL:HB	1:B:1488:VAL:HG22	1.95	0.49
1:B:2065:TRP:CD1	1:B:2081:ARG:HG2	2.48	0.48
1:B:607:GLN:O	1:B:610:ARG:NH2	2.46	0.48
1:B:1841:LYS:O	1:B:1845:LEU:HG	2.13	0.48
1:B:933:PRO:HG3	1:B:943:LEU:HD22	1.96	0.48
1:B:1911:ASP:O	1:B:1915:ILE:HG12	2.13	0.48
1:B:1157:ASN:O	1:B:1161:ILE:HG12	2.14	0.48
1:B:1891:THR:HG23	1:B:1915:ILE:HD12	1.96	0.48
1:B:1900:SER:HB2	1:B:1902:MET:HE2	1.95	0.48
1:B:1138:GLU:O	1:B:1142:LYS:HG2	2.14	0.48
1:B:1627:MET:HE2	1:B:1627:MET:HB3	1.79	0.48
1:B:1153:LEU:HD22	1:B:1161:ILE:HD12	1.96	0.48
1:B:1862:HIS:CG	1:B:1863:HIS:N	2.79	0.48
1:B:1897:ALA:HA	1:B:1902:MET:HG3	1.96	0.48
2:J:2280:ASN:HB3	2:J:2309:HIS:CD2	2.49	0.48
1:B:1205:THR:HG23	1:B:1249:GLU:HG2	1.96	0.48
1:B:1222:TRP:O	1:B:1270:VAL:HA	2.14	0.48
1:B:1190:LEU:HD21	1:B:1284:VAL:HG11	1.96	0.47
1:B:513:ALA:O	1:B:517:MET:HG3	2.14	0.47
1:B:542:ALA:O	1:B:589:THR:HA	2.13	0.47
1:B:1712:ASP:HB3	6:B:5992:HOH:O	2.14	0.47
1:B:709:TYR:OH	1:B:745:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1113:ASN:O	1:B:1117:MET:HG3	2.14	0.47
1:B:429:GLN:O	4:B:5807:EDO:H21	2.14	0.47
1:B:1748:LYS:NZ	1:B:1807:GLU:O	2.36	0.47
1:B:2064:TRP:CZ3	1:B:2110:SER:HB3	2.50	0.47
1:B:2067:VAL:HB	1:B:2107:TYR:HB2	1.95	0.47
1:B:502:CYS:HA	1:B:652:SER:O	2.15	0.47
1:B:526:ASN:HB2	1:B:528:ASP:OD1	2.15	0.47
1:B:1018:PHE:HE1	1:B:1088:ALA:HA	1.79	0.47
2:J:2189:SER:HB2	2:J:2192:ASP:H	1.80	0.47
1:B:489:TYR:HB2	1:B:515:MET:HE1	1.97	0.47
1:B:543:PRO:HD2	1:B:547:LEU:HD23	1.97	0.47
1:B:1271:VAL:HG12	1:B:1279:GLU:HB2	1.97	0.47
1:B:609:VAL:O	1:B:610:ARG:NH1	2.48	0.46
1:B:752:LEU:HB3	1:B:759:THR:HG22	1.96	0.46
1:B:850:LEU:HD23	1:B:883:LEU:HD23	1.98	0.46
1:B:1961:LYS:HG2	1:B:1971:ILE:HD11	1.97	0.46
1:B:442:TYR:CD2	1:B:707:ILE:HD11	2.51	0.46
2:J:2149:PRO:O	2:J:2160:PRO:HD3	2.16	0.46
1:B:984:LEU:CD1	1:B:998:VAL:HB	2.45	0.46
1:B:1453:VAL:HG22	1:B:1456:VAL:HG22	1.98	0.46
1:B:1225:VAL:HG11	1:B:1256:VAL:HG11	1.98	0.46
1:B:654:THR:HG21	1:B:676:PHE:O	2.16	0.45
1:B:2077:ILE:HG13	1:B:2094:PHE:CZ	2.52	0.45
1:B:1335:VAL:O	1:B:1339:VAL:HG23	2.17	0.45
1:B:2105:THR:HG22	1:B:2121:LYS:HG2	1.97	0.45
1:B:580:ILE:HG23	1:B:586:ILE:HD11	1.98	0.45
1:B:757:ALA:O	1:B:761:VAL:HG23	2.16	0.45
1:B:1009:LEU:HG	1:B:1013:GLU:HB3	1.98	0.45
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.98	0.45
1:B:1824:ILE:HD13	1:B:1922:LEU:HD23	1.98	0.45
1:B:1022:SER:O	1:B:1025:LYS:HB2	2.16	0.45
1:B:1041:LEU:HD11	1:B:1048:VAL:HB	1.98	0.45
1:B:1772:ASN:O	1:B:1772:ASN:ND2	2.50	0.45
1:B:461:LEU:HB3	1:B:480:THR:OG1	2.16	0.45
1:B:771:ASN:O	1:B:775:LYS:N	2.43	0.45
1:B:1122:MET:HE3	1:B:1122:MET:HB2	1.90	0.45
1:B:1664:MET:O	1:B:1705:MET:HB2	2.17	0.45
1:B:1258:VAL:HG12	1:B:1259:PHE:H	1.83	0.44
1:B:1566:ARG:HG3	1:B:1621:HIS:CG	2.52	0.44
2:J:2147:MET:O	2:J:2274:PRO:HD3	2.17	0.44
1:B:1259:PHE:CE2	4:B:5806:EDO:H22	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:LYS:HE3	1:B:861:TYR:CE2	2.53	0.44
1:B:929:MET:HE3	1:B:949:LEU:HD13	1.99	0.44
1:B:1228:VAL:HG13	4:B:5806:EDO:H12	1.99	0.44
2:J:2280:ASN:HB3	2:J:2309:HIS:CG	2.52	0.44
1:B:715:HIS:CD2	1:B:825:THR:HG21	2.53	0.44
1:B:1006:LYS:H	1:B:1009:LEU:HD13	1.83	0.44
1:B:726:HIS:NE2	1:B:830:GLY:O	2.47	0.44
1:B:1183:LYS:HG2	1:B:1207:ASP:HB3	2.00	0.44
1:B:1307:LEU:HD23	1:B:1328:PHE:CD2	2.52	0.44
1:B:1456:VAL:HG23	1:B:1490:LEU:O	2.18	0.44
1:B:1514:PHE:HB3	1:B:1518:VAL:CG2	2.40	0.44
1:B:1123:TRP:HD1	1:B:1126:MET:HE3	1.83	0.44
1:B:2103:ASN:HA	1:B:2123:SER:HA	1.99	0.44
1:B:983:GLU:CD	1:B:986:ARG:HH21	2.26	0.43
1:B:603:ARG:HH22	1:B:1861:ARG:HA	1.83	0.43
1:B:1146:LYS:HB3	1:B:1148:PHE:HD1	1.83	0.43
1:B:1187:SER:OG	1:B:1203:THR:HB	2.17	0.43
1:B:1440:LYS:NZ	1:B:1742:THR:O	2.39	0.43
1:B:1606:ASP:HB3	1:B:1609:LEU:HB3	2.00	0.43
1:B:1673:ILE:H	1:B:1673:ILE:HG13	1.66	0.43
1:B:2068:ILE:O	1:B:2076:LEU:HD12	2.18	0.43
1:B:2077:ILE:HG23	1:B:2094:PHE:CG	2.53	0.43
2:J:2098:LYS:NZ	2:J:2101:GLY:HA3	2.34	0.43
1:B:1964:PRO:HD2	1:B:2007:VAL:HA	1.99	0.43
1:B:1997:LEU:HD13	1:B:2004:ILE:HG12	1.99	0.43
1:B:708:VAL:HG21	1:B:829:LYS:HG3	2.01	0.43
1:B:1940:LEU:HA	1:B:1943:MET:HB2	2.00	0.43
1:B:769:CYS:SG	1:B:775:LYS:HE2	2.59	0.43
1:B:1375:ARG:HD3	1:B:1419:LEU:O	2.18	0.43
1:B:1745:ILE:HA	1:B:1750:ASP:HB3	2.00	0.43
1:B:1927:VAL:O	1:B:1931:SER:OG	2.24	0.43
1:B:1044:VAL:O	2:J:2074:ARG:NH1	2.46	0.43
1:B:1357:THR:O	1:B:1361:GLU:HG3	2.19	0.43
2:J:2229:LYS:O	2:J:2256:TYR:HA	2.18	0.43
1:B:1071:LYS:HD3	1:B:1071:LYS:HA	1.73	0.42
1:B:621:HIS:HB2	1:B:889:ILE:HG23	2.02	0.42
1:B:1368:LEU:HD22	1:B:1403:LYS:HE3	2.02	0.42
1:B:1406:VAL:HG21	1:B:1418:LEU:HB3	2.00	0.42
1:B:1574:ILE:HD11	1:B:1608:THR:HG21	2.01	0.42
1:B:1625:SER:HB2	1:B:1628:GLU:HG3	2.01	0.42
1:B:1899:LEU:HA	1:B:1899:LEU:HD23	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2306:HIS:ND1	2:J:2308:VAL:HG22	2.34	0.42
1:B:1018:PHE:CE2	1:B:1063:LEU:HD22	2.54	0.42
1:B:1223:ILE:O	1:B:1236:HIS:HA	2.19	0.42
1:B:1535:THR:HG21	1:B:1676:TYR:CE2	2.54	0.42
1:B:1269:ARG:HD2	1:B:1279:GLU:OE2	2.19	0.42
1:B:1590:LEU:HD22	1:B:1614:LEU:O	2.19	0.42
1:B:1735:HIS:O	1:B:1739:GLU:HG2	2.19	0.42
1:B:635:ALA:O	1:B:639:ILE:HG13	2.20	0.42
1:B:1225:VAL:HG21	1:B:1254:PHE:CE1	2.54	0.42
1:B:1515:HIS:O	1:B:1517:ASN:N	2.53	0.42
1:B:542:ALA:HB3	1:B:548:VAL:HG23	2.01	0.42
1:B:1553:HIS:HB3	1:B:1701:ARG:HD2	2.00	0.42
1:B:1836:LEU:HD23	1:B:1848:ILE:HD13	2.01	0.42
1:B:1933:ASN:HB3	1:B:1935:TRP:CD1	2.54	0.42
1:B:1945:LEU:HD13	1:B:1948:MET:HE2	2.01	0.42
1:B:2076:LEU:HD11	1:B:2079:ILE:HG23	2.01	0.42
1:B:695:LYS:HD3	1:B:695:LYS:HA	1.66	0.42
1:B:988:ALA:HB2	1:B:998:VAL:HG21	2.02	0.42
1:B:1356:LYS:HB2	1:B:1356:LYS:HE2	1.89	0.42
1:B:1132:PHE:HE1	1:B:1214:VAL:HG11	1.84	0.42
1:B:1589:PHE:HB3	1:B:1642:GLN:HB3	2.01	0.42
1:B:2093:ASP:OD1	1:B:2093:ASP:N	2.53	0.42
2:J:2303:GLU:H	2:J:2303:GLU:CD	2.27	0.42
1:B:813:ALA:HB2	1:B:852:MET:HE2	2.02	0.41
1:B:1957:ASP:HB3	1:B:1961:LYS:HD2	2.02	0.41
2:J:2090:ILE:HG21	2:J:2111:LEU:HD21	2.01	0.41
1:B:1129:LEU:HD23	1:B:1129:LEU:HA	1.80	0.41
1:B:1725:GLU:HB3	1:B:1771:TYR:OH	2.19	0.41
1:B:827:ILE:HG12	1:B:868:ILE:HB	2.03	0.41
1:B:1960:LEU:HD12	1:B:1971:ILE:HG23	2.03	0.41
2:J:2216:CYS:HA	2:J:2225:LEU:HD23	2.03	0.41
1:B:984:LEU:HD12	1:B:998:VAL:HB	2.03	0.41
1:B:1494:LEU:O	1:B:1513:ASN:ND2	2.50	0.41
1:B:1666:THR:HG21	1:B:1714:PHE:CE2	2.56	0.41
1:B:1858:ILE:HG12	1:B:1915:ILE:HD11	2.01	0.41
1:B:1093:ARG:NH2	1:B:1273:ASP:OD1	2.53	0.41
1:B:1321:TYR:OH	1:B:1361:GLU:OE1	2.28	0.41
1:B:1910:SER:O	1:B:1914:GLU:HG2	2.21	0.41
1:B:1957:ASP:N	1:B:1957:ASP:OD1	2.53	0.41
1:B:1375:ARG:HH21	1:B:1447:ASN:CB	2.34	0.41
1:B:488:LEU:HD22	1:B:501:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:ASP:O	1:B:977:GLY:N	2.51	0.41
1:B:1567:LYS:O	1:B:1571:LEU:HG	2.21	0.41
1:B:694:GLU:HG2	1:B:699:LYS:CG	2.50	0.41
1:B:770:LYS:HE3	1:B:793:ASP:OD1	2.21	0.41
1:B:1733:HIS:HB3	1:B:1796:LEU:HD21	2.02	0.41
1:B:1875:VAL:HG12	1:B:1877:HIS:HB3	2.03	0.41
1:B:1912:THR:O	1:B:1916:LEU:HG	2.21	0.41
1:B:666:ARG:HA	6:B:5948:HOH:O	2.20	0.40
1:B:2077:ILE:HG23	1:B:2094:PHE:CD1	2.56	0.40
2:J:2084:HIS:O	2:J:2087:THR:OG1	2.37	0.40
1:B:509:LYS:HD2	1:B:651:LEU:HB3	2.02	0.40
1:B:1174:ILE:O	1:B:1178:VAL:HG23	2.20	0.40
1:B:1200:VAL:O	1:B:1253:THR:HA	2.20	0.40
1:B:1515:HIS:NE2	1:B:1721:PRO:HG3	2.36	0.40
1:B:2099:THR:HG22	1:B:2126:VAL:HG11	2.04	0.40
1:B:2109:MET:HE2	1:B:2109:MET:HB3	1.92	0.40
1:B:1419:LEU:HG	1:B:1444:ASN:HB3	2.03	0.40
1:B:1953:MET:HE3	1:B:2114:MET:SD	2.61	0.40
1:B:403:LEU:HB2	1:B:954:LEU:CD1	2.50	0.40
1:B:626:PRO:HB2	1:B:896:LYS:HD2	2.03	0.40
1:B:1092:MET:SD	1:B:1114:LEU:HD23	2.61	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:B:1720:GLU:OE2	1:B:2000:THR:OG1[3_554]	2.12	0.08

## 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	1723/1747 (99%)	1658 (96%)	61 (4%)	4 (0%)	43 72
2	J	261/263 (99%)	247 (95%)	12 (5%)	2 (1%)	16 44
All	All	1984/2010 (99%)	1905 (96%)	73 (4%)	6 (0%)	36 66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	657	ASN
2	J	2135	ASP
1	B	1863	HIS
2	J	2059	PRO
1	B	1326	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	1544/1560 (99%)	1474 (96%)	70 (4%)	24 58
2	J	236/236 (100%)	226 (96%)	10 (4%)	26 61
All	All	1780/1796 (99%)	1700 (96%)	80 (4%)	24 58

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	418	GLN
1	B	459	GLU
1	B	489	TYR
1	B	546	SER
1	B	548	VAL
1	B	550	GLU
1	B	561	THR
1	B	585	ILE
1	B	602	GLU
1	B	617	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	627	VAL
1	B	720	GLN
1	B	727	SER
1	B	728	ARG
1	B	747	THR
1	B	835	SER
1	B	914	LYS
1	B	954	LEU
1	B	969	LEU
1	B	970	VAL
1	B	984	LEU
1	B	998	VAL
1	B	1009	LEU
1	B	1087	SER
1	B	1188	VAL
1	B	1228	VAL
1	B	1251	LEU
1	B	1258	VAL
1	B	1274	ARG
1	B	1277	SER
1	B	1357	THR
1	B	1358	ILE
1	B	1371	SER
1	B	1395	GLU
1	B	1402	ASN
1	B	1411	GLU
1	B	1412	THR
1	B	1458	LEU
1	B	1469	VAL
1	B	1537	THR
1	B	1559	VAL
1	B	1596	ASP
1	B	1598	ILE
1	B	1673	ILE
1	B	1699	GLU
1	B	1729	ASP
1	B	1731	CYS
1	B	1788	LEU
1	B	1797	GLU
1	B	1829	ILE
1	B	1831	LEU
1	B	1857	ASN

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Mol	Chain	Res	Type
1	B	1858	ILE
1	B	1861	ARG
1	B	1926	CYS
1	B	1927	VAL
1	B	1937	SER
1	B	1966	PHE
1	B	1979	VAL
1	B	1980	GLU
1	B	1994	ASN
1	B	1998	GLN
1	B	2013	ARG
1	B	2017	ILE
1	B	2047	VAL
1	B	2055	LEU
1	B	2068	ILE
1	B	2079	ILE
1	B	2082	LEU
1	B	2084	LEU
2	J	2066	THR
2	J	2098	LYS
2	J	2121	ARG
2	J	2147	MET
2	J	2156	THR
2	J	2189	SER
2	J	2212	ILE
2	J	2223	CYS
2	J	2226	THR
2	J	2239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	715	HIS
1	B	832	GLN
1	B	860	GLN
1	B	1026	ASN
1	B	1175	HIS
1	B	1191	GLN
1	B	1568	GLN
1	B	1615	ASN
1	B	1772	ASN
1	B	1903	GLN

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Mol	Chain	Res	Type
1	B	1947	GLN
1	B	1962	GLN
2	J	2165	GLN
2	J	2297	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

12 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	Q96	B	5802	-	14,14,14	2.97	6 (42%)	20,20,20	3.69	8 (40%)
4	EDO	B	5805	-	3,3,3	0.50	0	2,2,2	0.43	0
4	EDO	B	5807	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	B	5810	-	3,3,3	0.46	0	2,2,2	0.32	0
5	GOL	B	5804	-	5,5,5	1.31	1 (20%)	5,5,5	0.79	0
4	EDO	B	5811	-	3,3,3	0.57	0	2,2,2	0.06	0
3	Q96	B	5801	-	14,14,14	2.87	6 (42%)	20,20,20	3.86	8 (40%)
4	EDO	B	5809	-	3,3,3	0.58	0	2,2,2	0.02	0
4	EDO	B	5803	-	3,3,3	0.41	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	B	5808	-	3,3,3	0.41	0	2,2,2	0.69	0
4	EDO	B	5806	-	3,3,3	0.50	0	2,2,2	0.25	0
4	EDO	B	5812	-	3,3,3	0.44	0	2,2,2	0.21	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	Q96	B	5802	-	-	5/11/11/11	0/1/1/1
4	EDO	B	5805	-	-	1/1/1/1	-
4	EDO	B	5807	-	-	0/1/1/1	-
4	EDO	B	5810	-	-	0/1/1/1	-
5	GOL	B	5804	-	-	4/4/4/4	-
4	EDO	B	5811	-	-	1/1/1/1	-
3	Q96	B	5801	-	-	2/11/11/11	0/1/1/1
4	EDO	B	5809	-	-	0/1/1/1	-
4	EDO	B	5803	-	-	0/1/1/1	-
4	EDO	B	5808	-	-	1/1/1/1	-
4	EDO	B	5806	-	-	1/1/1/1	-
4	EDO	B	5812	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5801	Q96	S10-N13	7.51	1.72	1.61
3	B	5802	Q96	S10-N13	7.17	1.72	1.61
3	B	5802	Q96	C03-N02	4.65	1.46	1.37
3	B	5801	Q96	C03-N02	4.36	1.45	1.37
3	B	5802	Q96	C07-S10	3.78	1.82	1.76
3	B	5802	Q96	O11-S10	3.72	1.47	1.43
3	B	5802	Q96	O12-S10	3.64	1.47	1.43
3	B	5801	Q96	O12-S10	3.53	1.47	1.43
3	B	5801	Q96	C07-S10	3.35	1.81	1.76
3	B	5801	Q96	O11-S10	3.02	1.47	1.43
3	B	5802	Q96	C04-N05	2.65	1.46	1.38
3	B	5801	Q96	C04-N05	2.50	1.46	1.38
5	B	5804	GOL	O2-C2	-2.03	1.37	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5801	Q96	O12-S10-O11	-14.98	101.33	119.52
3	B	5802	Q96	O12-S10-O11	-13.45	103.19	119.52
3	B	5802	Q96	C09-C03-N02	-4.30	115.97	121.33
3	B	5802	Q96	C04-C03-N02	4.08	123.49	118.30
3	B	5802	Q96	C01-N02-C03	-3.60	116.70	122.37
3	B	5801	Q96	C09-C03-N02	-3.42	117.07	121.33
3	B	5801	Q96	C04-C03-N02	3.38	122.60	118.30
3	B	5801	Q96	O11-S10-N13	3.30	113.15	107.06
3	B	5801	Q96	C01-N02-C03	-3.26	117.23	122.37
3	B	5802	Q96	C06-C07-S10	3.08	122.21	119.06
3	B	5801	Q96	C14-N13-S10	2.98	123.11	119.16
3	B	5802	Q96	O12-S10-N13	2.96	112.51	107.06
3	B	5802	Q96	C07-S10-N13	2.63	111.16	107.55
3	B	5802	Q96	C08-C07-S10	-2.47	117.04	119.76
3	B	5801	Q96	O12-S10-C07	2.40	111.00	107.98
3	B	5801	Q96	O11-S10-C07	2.34	110.93	107.98

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5801	Q96	C14-N13-S10-C07
3	B	5801	Q96	C14-N13-S10-O11
3	B	5802	Q96	C14-N13-S10-O12
5	B	5804	GOL	O1-C1-C2-O2
5	B	5804	GOL	O1-C1-C2-C3
5	B	5804	GOL	C1-C2-C3-O3
3	B	5802	Q96	C08-C07-S10-O11
3	B	5802	Q96	C06-C07-S10-O11
3	B	5802	Q96	C06-C07-S10-N13
3	B	5802	Q96	C08-C07-S10-N13
5	B	5804	GOL	O2-C2-C3-O3
4	B	5805	EDO	O1-C1-C2-O2
4	B	5808	EDO	O1-C1-C2-O2
4	B	5811	EDO	O1-C1-C2-O2
4	B	5806	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

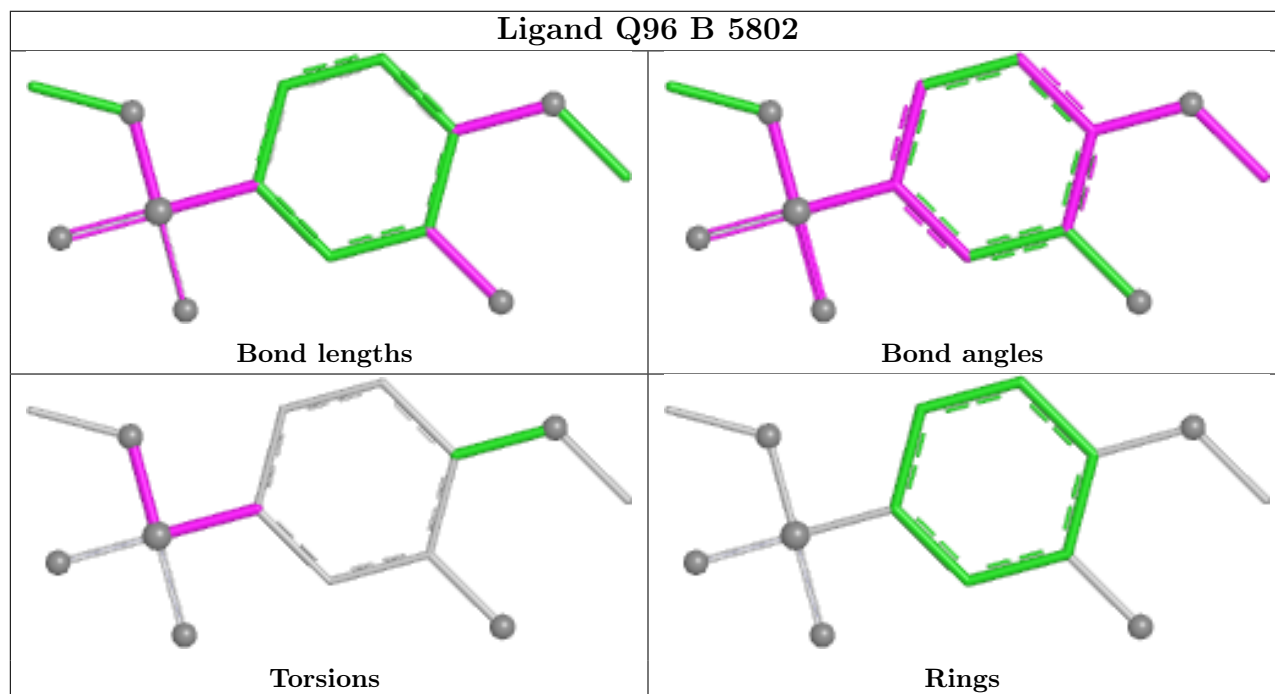
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5807	EDO	1	0

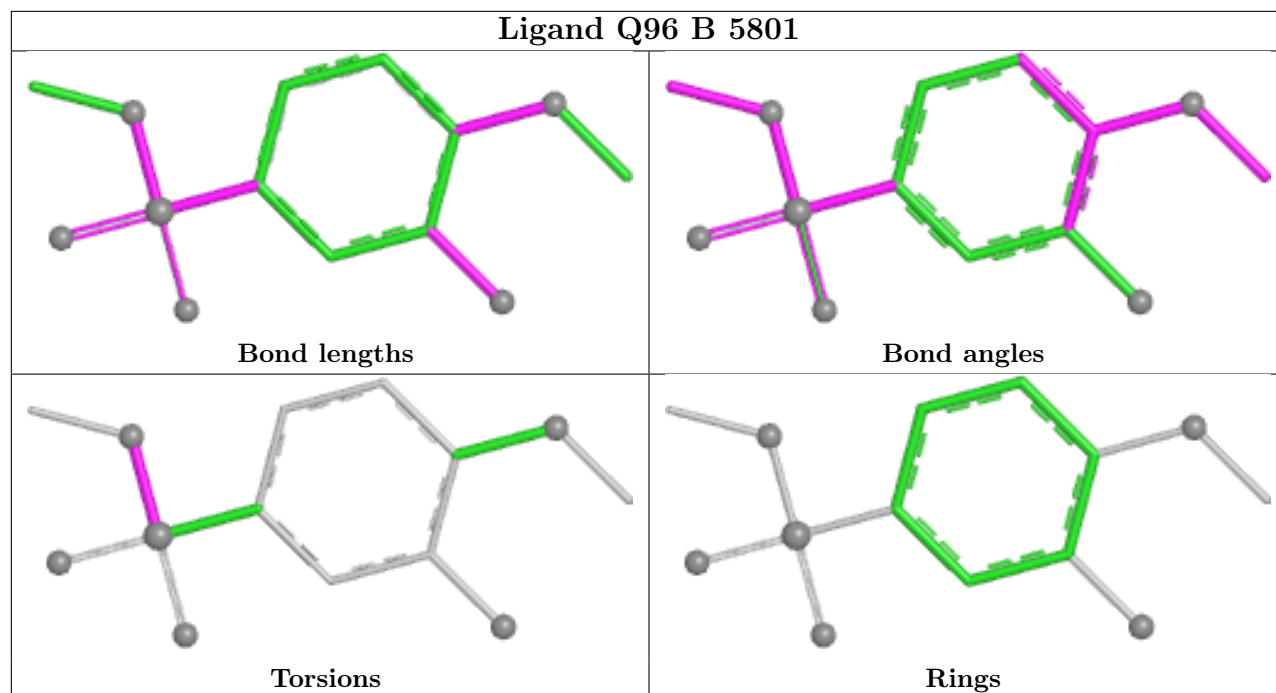
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5806	EDO	4	0
4	B	5812	EDO	1	0

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	1724/1747 (98%)	0.02	30 (1%) 69 60	40, 70, 147, 263	1 (0%)
2	J	263/263 (100%)	-0.12	3 (1%) 78 70	44, 66, 141, 186	0
All	All	1987/2010 (98%)	0.00	33 (1%) 69 60	40, 69, 146, 263	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	HIS	4.4
2	J	2318	ALA	3.8
1	B	1501	ALA	3.5
1	B	1360	ALA	3.4
2	J	2317	PHE	3.3
1	B	1584	ILE	3.2
1	B	1996	LEU	3.1
1	B	1868	LEU	3.0
1	B	1755	LEU	2.9
2	J	2060	LEU	2.9
1	B	1979	VAL	2.7
1	B	1044	VAL	2.7
1	B	1308	PRO	2.7
1	B	1617	VAL	2.7
1	B	1135	LEU	2.6
1	B	704	MET	2.5
1	B	1904	LEU	2.5
1	B	1926	CYS	2.5
1	B	604	THR	2.4
1	B	1328	PHE	2.4
1	B	1879	LEU	2.3
1	B	1862	HIS	2.3
1	B	970	VAL	2.3
1	B	1499	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1849	ILE	2.2
1	B	1971	ILE	2.2
1	B	1336	PHE	2.2
1	B	1061	VAL	2.2
1	B	1882	PRO	2.1
1	B	1307	LEU	2.1
1	B	1985	ILE	2.1
1	B	1960	LEU	2.1
1	B	734	THR	2.1

## 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.

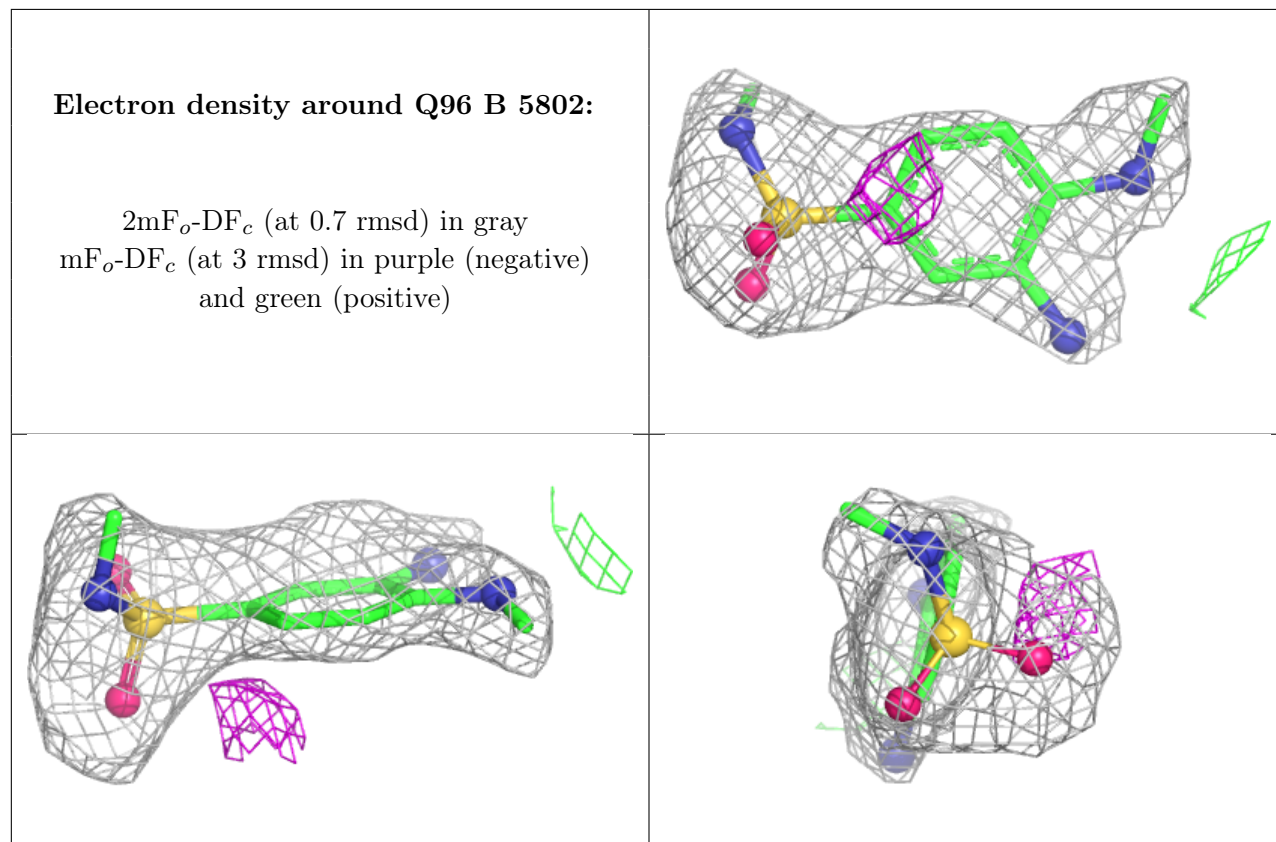
## 6.4 Ligands [i](#)

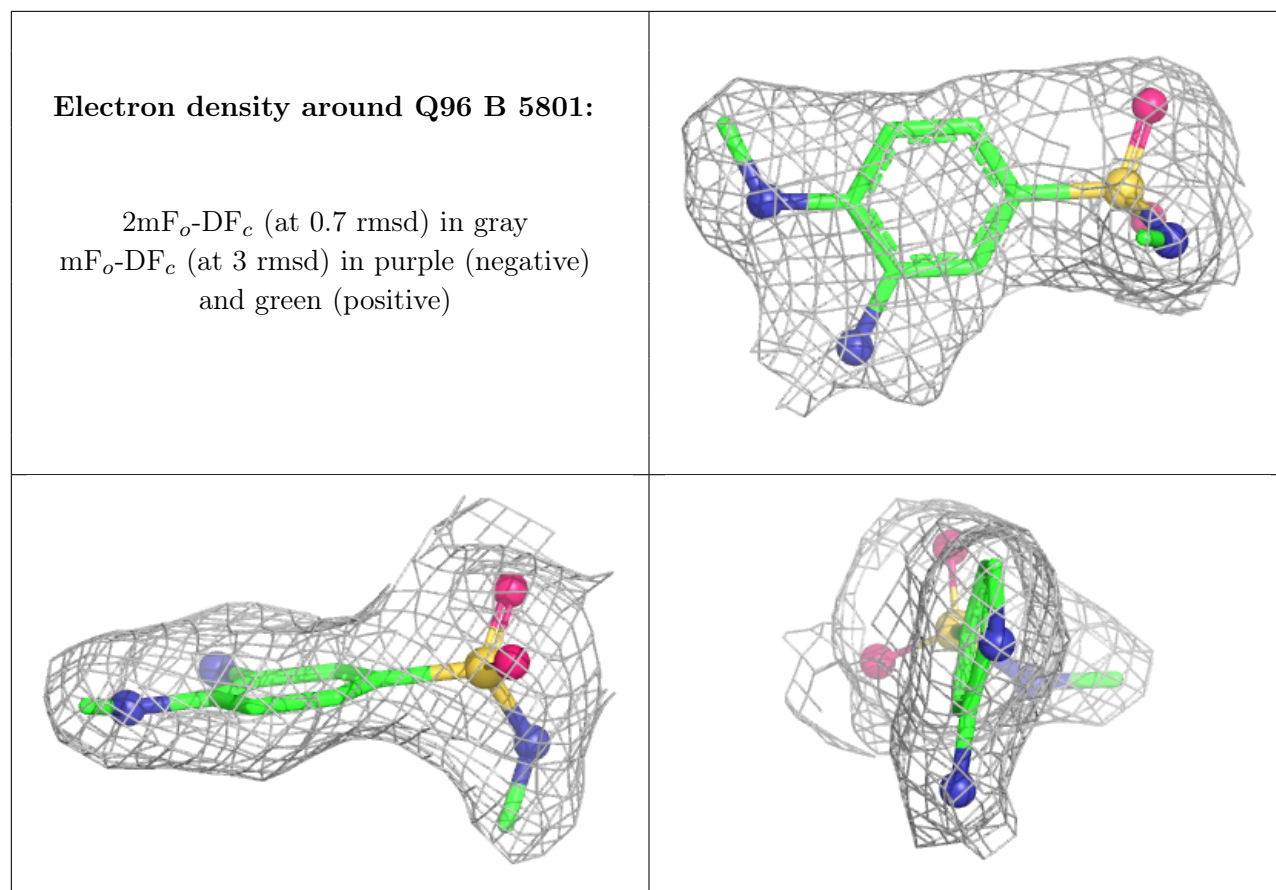
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	5810	4/4	0.64	0.13	81,88,94,97	0
4	EDO	B	5807	4/4	0.74	0.10	70,71,73,73	0
4	EDO	B	5805	4/4	0.79	0.15	56,58,62,64	0
4	EDO	B	5806	4/4	0.80	0.15	55,60,63,63	0
3	Q96	B	5802	14/14	0.83	0.10	43,61,83,88	0
4	EDO	B	5812	4/4	0.85	0.09	70,73,75,76	0
4	EDO	B	5808	4/4	0.88	0.14	50,53,55,63	0
5	GOL	B	5804	6/6	0.88	0.14	48,62,64,65	0
4	EDO	B	5809	4/4	0.89	0.11	59,61,65,66	0
4	EDO	B	5811	4/4	0.93	0.08	67,68,68,70	0
3	Q96	B	5801	14/14	0.93	0.08	45,52,58,59	0
4	EDO	B	5803	4/4	0.93	0.08	45,46,48,52	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.