



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:06 AM UTC

PDB ID : 8BC8 / pdb_00008bc8
Title : Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and compound 18
Authors : Vester, K.; Loll, B.; Wahl, M.C.
Deposited on : 2022-10-15
Resolution : 2.39 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

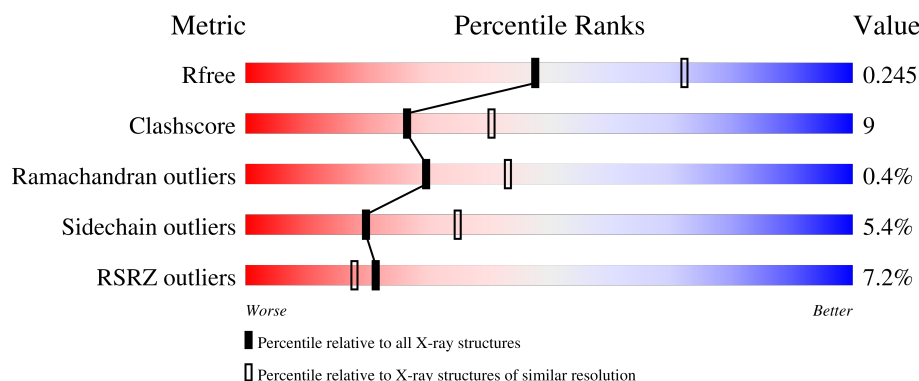
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	B	1747	7% 74% 23% ..
2	J	263	5% 80% 18% .

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	QB6	B	5802	-	X	-	-
3	QB6	B	5803	-	X	-	-
3	QB6	J	2402	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16467 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	13901	8881	2381	2567	72	0	4	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

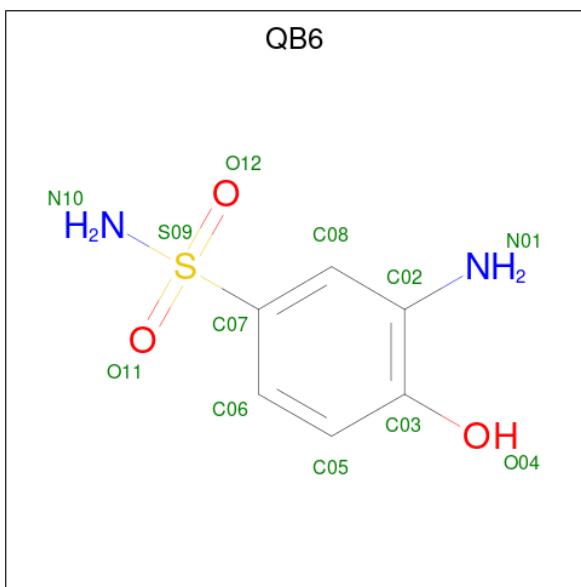
- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

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:

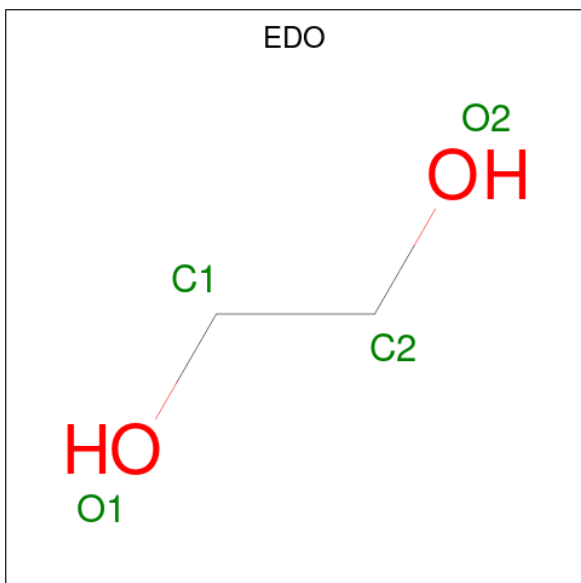
Chain	Residue	Modelled	Actual	Comment	Reference
J	2058	GLY	-	expression tag	UNP Q6P2Q9
J	2059	PRO	-	expression tag	UNP Q6P2Q9
J	2060	LEU	-	expression tag	UNP Q6P2Q9
J	2061	GLY	-	expression tag	UNP Q6P2Q9
J	2062	SER	-	expression tag	UNP Q6P2Q9
J	2063	MET	-	expression tag	UNP Q6P2Q9

- Molecule 3 is 3-azanyl-4-oxidanyl-benzenesulfonamide (CCD ID: QB6) (formula: $C_6H_8N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
3	J	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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
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	J	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0

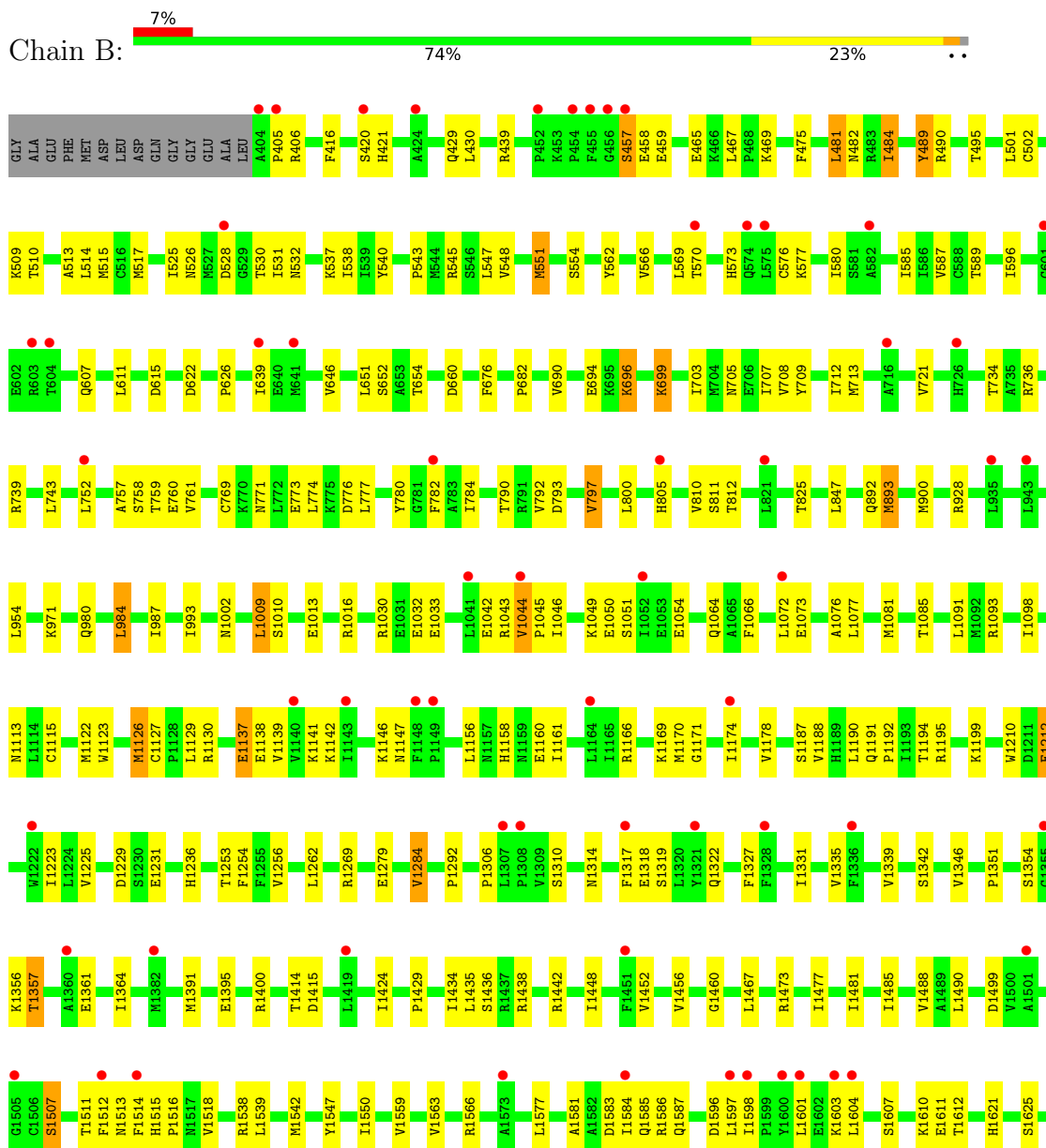
- Molecule 5 is water.

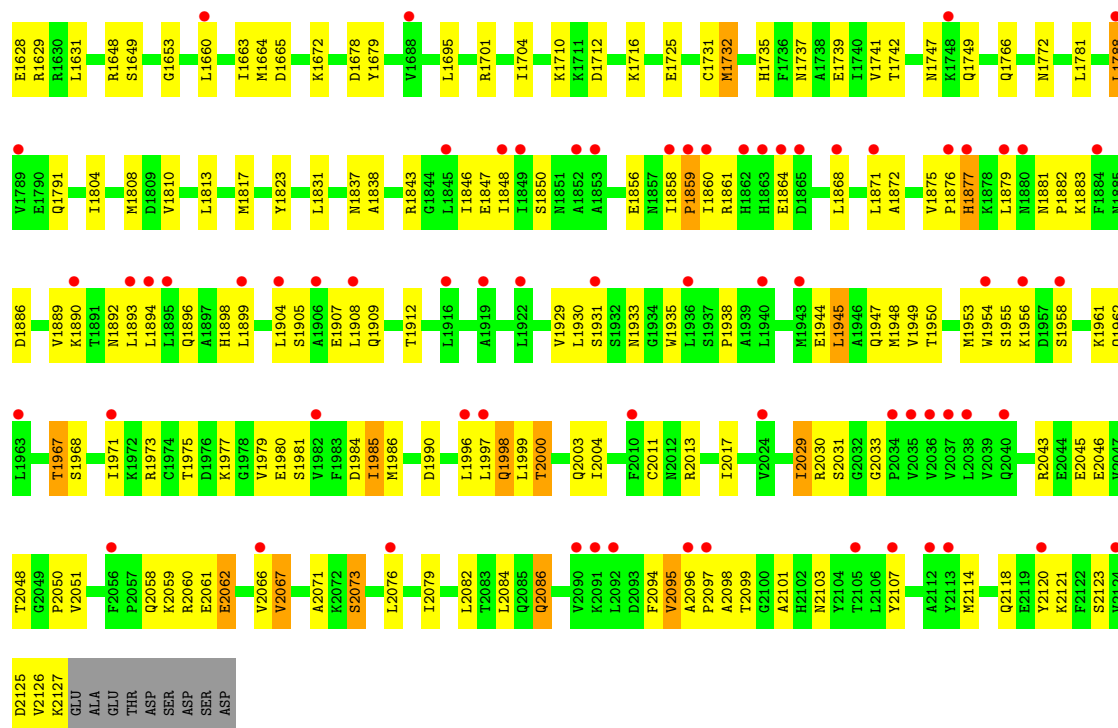
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	288	Total O 288 288	0	2
5	J	43	Total O 43 43	0	0

3 Residue-property plots [i](#)

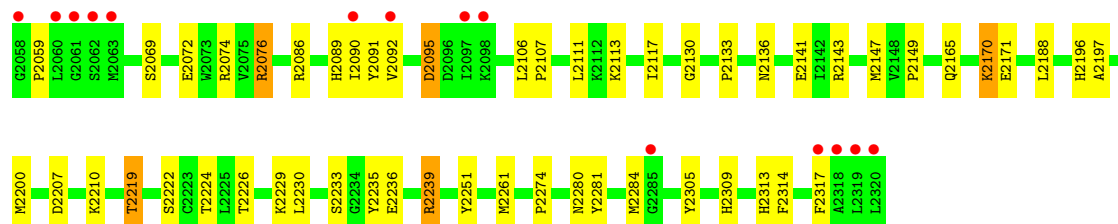
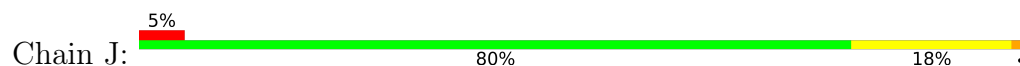
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	100.60Å 119.06Å 187.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.33 – 2.39 46.33 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.33-2.39) 99.9 (46.33-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.207 , 0.245 0.206 , 0.245	Depositor DCC
R_{free} test set	2100 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16467	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: QB6, 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	0.39	0/14196	0.55	0/19233
2	J	0.43	0/2190	0.60	0/2981
All	All	0.39	0/16386	0.56	0/22214

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

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	13901	0	14035	268	1
2	J	2123	0	2063	38	0
3	B	36	0	0	1	0
3	J	12	0	0	0	0
4	B	56	0	84	7	0
4	J	8	0	12	1	0
5	B	288	0	0	5	0
5	J	43	0	0	2	0
All	All	16467	0	16194	300	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 9.

All (300) 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:1542:MET:HE3	1:B:1664:MET:HG2	1.51	0.93
1:B:1253:THR:H	4:B:5816:EDO:H22	1.34	0.91
1:B:489:TYR:HB2	1:B:515:MET:HE1	1.62	0.81
1:B:1672:LYS:HG3	1:B:1859:PRO:HB3	1.61	0.80
1:B:1010:SER:OG	1:B:1013:GLU:OE1	2.01	0.78
2:J:2141:GLU:OE1	2:J:2143:ARG:NH2	2.18	0.77
1:B:570:THR:OG1	1:B:576:CYS:SG	2.42	0.76
1:B:2067:VAL:HG13	1:B:2107:TYR:HB2	1.70	0.74
1:B:708:VAL:O	1:B:712:ILE:HG12	1.90	0.72
1:B:993:ILE:HD12	1:B:1091:LEU:HD23	1.69	0.71
1:B:1894:LEU:HG	1:B:1912:THR:HG22	1.71	0.71
1:B:1628:GLU:HA	1:B:1631:LEU:HD12	1.73	0.71
2:J:2072:GLU:HG2	2:J:2076:ARG:HH21	1.56	0.71
1:B:1195:ARG:H	4:B:5810:EDO:H22	1.56	0.70
1:B:2017:ILE:HG12	1:B:2043:ARG:HD2	1.74	0.70
2:J:2133:PRO:HG2	2:J:2136:ASN:HB3	1.74	0.69
1:B:1229:ASP:HB2	1:B:1231:GLU:HG2	1.74	0.69
2:J:2196:HIS:HD2	2:J:2200:MET:HE2	1.58	0.68
1:B:984:LEU:HD21	1:B:1002:ASN:HB2	1.76	0.68
1:B:626:PRO:HB3	1:B:893:MET:HE3	1.76	0.67
1:B:1843:ARG:HH12	1:B:1876:PRO:HB2	1.61	0.66
2:J:2196:HIS:CD2	2:J:2200:MET:HE2	2.30	0.66
2:J:2092:VAL:HG13	2:J:2261:MET:HE3	1.77	0.65
1:B:537:LYS:NZ	1:B:580:ILE:O	2.29	0.65
1:B:1126:MET:HB3	1:B:1130:ARG:HD2	1.77	0.65
4:B:5813:EDO:O2	5:B:5901:HOH:O	2.15	0.64
1:B:1877:HIS:CE1	1:B:1879:LEU:HD23	2.33	0.64
2:J:2236:GLU:OE2	2:J:2239:ARG:NH1	2.30	0.64
1:B:1629:ARG:NH2	1:B:1653:GLY:O	2.31	0.63
1:B:543:PRO:HD2	1:B:547:LEU:HD23	1.81	0.63
1:B:1188:VAL:HG21	1:B:1284:VAL:HG13	1.80	0.63
1:B:1604:LEU:HD23	1:B:1628:GLU:HG2	1.80	0.63
1:B:1868:LEU:HB3	1:B:1893:LEU:HD13	1.80	0.63
1:B:790:THR:HG22	1:B:792:VAL:H	1.64	0.62
1:B:654:THR:HG21	1:B:676:PHE:O	1.98	0.62
1:B:1886:ASP:O	1:B:1889:VAL:HG12	1.99	0.62
1:B:1030:ARG:HH21	1:B:1076:ALA:HB1	1.65	0.62
1:B:1507:SER:O	1:B:1511:THR:HG23	1.99	0.62
1:B:1586:ARG:HD2	1:B:1587:GLN:H	1.64	0.62
1:B:1127:CYS:O	1:B:1130:ARG:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1009:LEU:HG	1:B:1013:GLU:HB2	1.81	0.62
1:B:1156:LEU:HB2	1:B:1161:ILE:HG13	1.81	0.61
2:J:2147:MET:O	2:J:2274:PRO:HD3	1.99	0.61
1:B:1747:ASN:HB2	1:B:1808:MET:HE3	1.83	0.61
1:B:1030:ARG:O	1:B:1033:GLU:HG2	2.01	0.61
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.82	0.61
1:B:1892:ASN:O	1:B:1896:GLN:NE2	2.34	0.61
1:B:2043:ARG:HB2	1:B:2086:GLN:HA	1.82	0.61
1:B:1539:LEU:HD23	1:B:1542:MET:HE2	1.83	0.60
1:B:540:TYR:CE1	1:B:551:MET:HE3	2.37	0.60
1:B:893:MET:HE1	1:B:900:MET:HG3	1.83	0.59
1:B:1732:MET:HE2	1:B:1788:LEU:HD12	1.83	0.59
1:B:1861:ARG:HG2	1:B:1864:GLU:H	1.67	0.59
1:B:1804:ILE:HG12	1:B:1810:VAL:HG12	1.85	0.59
1:B:2051:VAL:HG22	1:B:2062:GLU:HG2	1.85	0.59
1:B:694:GLU:HG2	1:B:699:LYS:HB3	1.85	0.58
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	1.85	0.58
1:B:1678:ASP:OD1	1:B:1710:LYS:HE3	2.04	0.58
1:B:1898:HIS:HD2	1:B:1899:LEU:HD12	1.68	0.58
1:B:712:ILE:HD12	1:B:721:VAL:HG21	1.85	0.57
1:B:1950:THR:HG21	1:B:2060:ARG:HH21	1.70	0.57
1:B:484:ILE:HD11	1:B:501:LEU:HD21	1.86	0.57
1:B:1846:ILE:HD11	1:B:1945:LEU:HD21	1.86	0.57
1:B:1861:ARG:HD3	1:B:1864:GLU:HB2	1.85	0.57
1:B:1864:GLU:O	1:B:1868:LEU:HG	2.04	0.57
1:B:1881:ASN:HD22	1:B:1883:LYS:NZ	2.03	0.57
1:B:1944:GLU:HG3	1:B:1948:MET:HE3	1.87	0.56
2:J:2207:ASP:HB3	2:J:2210:LYS:HB2	1.87	0.56
1:B:1190:LEU:HD21	1:B:1284:VAL:HG11	1.87	0.56
1:B:1846:ILE:O	1:B:1850:SER:OG	2.19	0.56
1:B:482:ASN:OD1	1:B:484:ILE:HG22	2.05	0.56
2:J:2106:LEU:HD12	2:J:2107:PRO:HD2	1.86	0.56
1:B:1566:ARG:HG2	1:B:1621:HIS:CG	2.41	0.56
1:B:2098:ALA:O	1:B:2126:VAL:HG21	2.06	0.56
1:B:1042:GLU:HG3	2:J:2069:SER:O	2.06	0.55
1:B:1456:VAL:HG12	1:B:1490:LEU:O	2.07	0.55
2:J:2106:LEU:HD21	2:J:2111:LEU:HD13	1.87	0.55
1:B:548:VAL:HG13	1:B:587:VAL:HG12	1.89	0.55
1:B:1837:ASN:OD1	1:B:1838:ALA:N	2.41	0.54
1:B:1843:ARG:HB3	1:B:1877:HIS:HB2	1.89	0.54
2:J:2281:TYR:HA	2:J:2284:MET:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1663:ILE:HD12	1:B:1704:ILE:HG12	1.90	0.54
1:B:1947:GLN:HB3	1:B:2114:MET:HG2	1.89	0.54
1:B:1429:PRO:HG3	1:B:1467:LEU:HD13	1.90	0.54
1:B:1586:ARG:HD2	1:B:1587:GLN:N	2.22	0.54
1:B:1843:ARG:HD2	1:B:1877:HIS:HB2	1.89	0.54
1:B:639:ILE:HD11	1:B:646:VAL:HB	1.90	0.54
1:B:2043:ARG:NH2	1:B:2062:GLU:OE1	2.40	0.54
1:B:1542:MET:HE1	1:B:1665:ASP:HB2	1.90	0.54
1:B:1933:ASN:HB3	1:B:1935:TRP:CE2	2.43	0.53
1:B:1044:VAL:O	2:J:2074:ARG:NH2	2.40	0.53
1:B:1364:ILE:HG21	1:B:1424:ILE:HD11	1.91	0.53
1:B:1542:MET:CE	1:B:1664:MET:HG2	2.31	0.53
1:B:1225:VAL:HG21	1:B:1254:PHE:CE1	2.44	0.53
1:B:526:ASN:ND2	1:B:532:ASN:OD1	2.42	0.53
1:B:1066:PHE:HD1	1:B:1081:MET:HE3	1.72	0.52
1:B:1156:LEU:HB3	1:B:1160:GLU:HB2	1.90	0.52
1:B:1954:TRP:HB2	1:B:1956:LYS:HE3	1.90	0.52
1:B:1868:LEU:HA	1:B:1871:LEU:HB3	1.90	0.52
1:B:1515:HIS:O	1:B:1518:VAL:HG22	2.08	0.52
1:B:2013:ARG:NH1	1:B:2048:THR:H	2.07	0.52
1:B:416:PHE:HB2	1:B:892:GLN:HE22	1.73	0.52
1:B:1319:SER:O	1:B:1400:ARG:NH1	2.43	0.52
2:J:2089:HIS:O	2:J:2222:SER:HB2	2.10	0.52
1:B:721:VAL:HG12	1:B:825:THR:HB	1.91	0.52
1:B:1174:ILE:O	1:B:1178:VAL:HG23	2.10	0.52
1:B:2030:ARG:NE	1:B:2127:LYS:HE3	2.25	0.52
1:B:1513:ASN:OD1	5:B:5902:HOH:O	2.19	0.52
1:B:1979:VAL:HG11	1:B:1985:ILE:HG22	1.92	0.52
1:B:2029:ILE:O	1:B:2127:LYS:N	2.43	0.52
2:J:2165:GLN:NE2	5:J:2503:HOH:O	2.39	0.52
2:J:2197:ALA:HA	2:J:2200:MET:HE3	1.91	0.51
4:J:2403:EDO:H21	5:J:2540:HOH:O	2.10	0.51
1:B:1539:LEU:HD22	1:B:1664:MET:HE3	1.93	0.51
1:B:531:ILE:HD13	1:B:562:TYR:O	2.11	0.51
1:B:547:LEU:O	1:B:551:MET:HG2	2.11	0.51
1:B:1515:HIS:CD2	1:B:1516:PRO:HD2	2.46	0.51
1:B:1712:ASP:OD2	1:B:1716:LYS:HE2	2.11	0.50
1:B:1045:PRO:HD3	2:J:2317:PHE:CD2	2.46	0.50
1:B:1547:TYR:OH	1:B:1583:ASP:OD2	2.25	0.50
1:B:1050:GLU:CD	1:B:1050:GLU:H	2.20	0.50
1:B:1357:THR:O	1:B:1361:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1438:ARG:HB2	1:B:1442:ARG:HD2	1.93	0.50
1:B:1890:LYS:O	1:B:1894:LEU:HB2	2.11	0.50
1:B:509:LYS:HB3	1:B:651:LEU:HD22	1.93	0.49
1:B:1130:ARG:NH2	1:B:1137:GLU:OE2	2.43	0.49
1:B:1997:LEU:HD12	1:B:1999:LEU:HB3	1.94	0.49
1:B:2101:ALA:HB1	1:B:2125:ASP:CG	2.36	0.49
1:B:739:ARG:HH22	1:B:776:ASP:CG	2.20	0.49
1:B:1123:TRP:HD1	1:B:1126:MET:HE1	1.77	0.49
1:B:406:ARG:HD3	1:B:954:LEU:HG	1.94	0.49
1:B:1043:ARG:HH22	2:J:2313:HIS:HA	1.76	0.49
1:B:589:THR:HG23	4:B:5804:EDO:H22	1.93	0.49
1:B:771:ASN:HB3	1:B:774:LEU:HB2	1.94	0.49
1:B:484:ILE:HD11	1:B:501:LEU:HD11	1.94	0.49
1:B:457:SER:O	1:B:459:GLU:N	2.45	0.49
1:B:566:VAL:HG13	1:B:585:ILE:HB	1.94	0.49
1:B:1139:VAL:HA	1:B:1142:LYS:HG3	1.93	0.49
1:B:811:SER:OG	1:B:812:THR:N	2.46	0.49
1:B:1043:ARG:HG3	2:J:2317:PHE:HD1	1.78	0.49
1:B:1672:LYS:HG3	1:B:1859:PRO:CB	2.37	0.49
2:J:2086:ARG:NH1	2:J:2219:THR:O	2.44	0.49
1:B:2071:ALA:C	1:B:2073:SER:H	2.21	0.48
1:B:1581:ALA:HA	1:B:1586:ARG:HD3	1.94	0.48
1:B:1813:LEU:O	1:B:1817:MET:HG3	2.14	0.48
1:B:1122:MET:SD	1:B:1130:ARG:HG3	2.54	0.48
1:B:777:LEU:HB3	1:B:782:PHE:O	2.13	0.48
1:B:1732:MET:CE	1:B:1788:LEU:HD12	2.43	0.48
1:B:1909:GLN:O	1:B:1912:THR:OG1	2.26	0.48
1:B:1434:ILE:HD13	1:B:1823:TYR:HB2	1.96	0.48
1:B:2030:ARG:HE	1:B:2127:LYS:HE3	1.77	0.48
1:B:1512:PHE:HB3	1:B:1514:PHE:CE2	2.49	0.47
1:B:421:HIS:ND1	5:B:5905:HOH:O	2.35	0.47
1:B:420:SER:HB3	1:B:622:ASP:HA	1.95	0.47
1:B:514:LEU:HA	1:B:517:MET:HE2	1.95	0.47
1:B:1583:ASP:CG	1:B:1584:ILE:H	2.20	0.47
1:B:1210:TRP:HE1	1:B:1212:GLU:HG3	1.80	0.47
1:B:2031:SER:HA	1:B:2096:ALA:HB3	1.96	0.47
1:B:2058:GLN:OE1	1:B:2058:GLN:N	2.48	0.47
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.54	0.47
1:B:475:PHE:CE2	1:B:481:LEU:HD22	2.50	0.47
1:B:757:ALA:O	1:B:761:VAL:HG23	2.15	0.47
1:B:2094:PHE:CZ	1:B:2097:PRO:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2076:ARG:HB3	2:J:2305:TYR:OH	2.14	0.47
1:B:1499:ASP:OD2	1:B:1766:GLN:HG3	2.15	0.46
1:B:1607:SER:O	1:B:1611:GLU:HG2	2.15	0.46
1:B:1138:GLU:O	1:B:1142:LYS:HG2	2.15	0.46
2:J:2280:ASN:HB3	2:J:2309:HIS:CG	2.50	0.46
1:B:1583:ASP:CG	1:B:1584:ILE:N	2.73	0.46
1:B:1191:GLN:OE1	1:B:1199:LYS:HE3	2.15	0.46
1:B:682:PRO:HG2	5:B:6122:HOH:O	2.16	0.46
1:B:987:ILE:HD13	1:B:1098:ILE:HG13	1.96	0.46
1:B:1452:VAL:HG22	1:B:1488:VAL:HB	1.98	0.46
1:B:1436:SER:O	1:B:1473:ARG:HD3	2.15	0.46
1:B:1905:SER:CB	1:B:1908:LEU:HB3	2.46	0.46
1:B:1905:SER:HB2	1:B:1908:LEU:HB3	1.98	0.46
1:B:1142:LYS:O	1:B:1146:LYS:HG2	2.16	0.46
1:B:1967:THR:HG22	1:B:1968:SER:H	1.81	0.46
1:B:1335:VAL:O	1:B:1339:VAL:HG23	2.15	0.46
2:J:2113:LYS:O	2:J:2117:ILE:HG23	2.16	0.46
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	1.98	0.46
1:B:1648:ARG:HD2	1:B:1679:TYR:CE1	2.52	0.45
1:B:1735:HIS:O	1:B:1739:GLU:HG2	2.16	0.45
1:B:2033:GLY:O	1:B:2095:VAL:HA	2.16	0.45
2:J:2133:PRO:HD3	2:J:2141:GLU:HG3	1.98	0.45
1:B:1049:LYS:HB2	1:B:1049:LYS:HE3	1.73	0.45
1:B:1127:CYS:SG	1:B:1129:LEU:HB2	2.57	0.45
1:B:790:THR:HG21	1:B:792:VAL:HG12	1.98	0.45
1:B:1169:LYS:O	1:B:1170:MET:HE2	2.16	0.45
1:B:1868:LEU:HD22	1:B:1871:LEU:HD22	1.98	0.45
1:B:1908:LEU:O	1:B:1912:THR:HG23	2.16	0.45
2:J:2188:LEU:O	2:J:2251:TYR:OH	2.33	0.45
1:B:2029:ILE:H	1:B:2127:LYS:HA	1.81	0.45
1:B:576:CYS:O	1:B:580:ILE:HG13	2.17	0.45
1:B:1093:ARG:NH1	1:B:1115:CYS:HB3	2.31	0.45
1:B:1314:ASN:HB3	1:B:1317:PHE:HB2	1.98	0.45
1:B:1986:MET:HE2	1:B:1986:MET:HB3	1.80	0.45
1:B:758:SER:HA	1:B:805:HIS:CD2	2.52	0.45
1:B:1146:LYS:NZ	1:B:1166:ARG:HG3	2.32	0.45
1:B:1583:ASP:OD1	1:B:1584:ILE:N	2.43	0.45
1:B:430:LEU:HD12	1:B:430:LEU:H	1.82	0.45
1:B:660:ASP:OD2	1:B:928:ARG:NH1	2.48	0.45
1:B:1395:GLU:O	1:B:1400:ARG:HG3	2.16	0.45
2:J:2229:LYS:NZ	2:J:2230:LEU:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1225:VAL:HG11	1:B:1256:VAL:HG11	1.98	0.45
1:B:1999:LEU:HB2	1:B:2004:ILE:HG23	1.99	0.45
1:B:1672:LYS:HZ1	1:B:1859:PRO:HD3	1.82	0.44
1:B:538:ILE:HG23	1:B:611:LEU:HD23	1.99	0.44
1:B:1945:LEU:O	1:B:1949:VAL:HG22	2.17	0.44
1:B:1538:ARG:O	1:B:1542:MET:HG3	2.17	0.44
1:B:548:VAL:HG11	4:B:5804:EDO:H12	1.99	0.44
1:B:1045:PRO:HB2	2:J:2314:PHE:CE2	2.53	0.44
1:B:1253:THR:N	4:B:5816:EDO:H22	2.17	0.44
1:B:1077:LEU:HD23	1:B:1077:LEU:HA	1.83	0.44
1:B:1550:ILE:HG12	1:B:1559:VAL:HG11	2.00	0.44
2:J:2095:ASP:N	2:J:2095:ASP:OD1	2.49	0.44
1:B:793:ASP:O	1:B:797:VAL:HG13	2.17	0.44
1:B:800:LEU:O	1:B:805:HIS:HB2	2.17	0.44
1:B:2066:VAL:O	1:B:2079:ILE:HA	2.17	0.44
2:J:2149:PRO:HD3	2:J:2274:PRO:HG3	2.00	0.44
2:J:2200:MET:HE1	2:J:2230:LEU:HD22	1.99	0.44
1:B:1306:PRO:HB2	1:B:1327:PHE:CD2	2.52	0.44
1:B:1660:LEU:HA	1:B:1701:ARG:O	2.18	0.43
1:B:573:HIS:O	1:B:577:LYS:HG2	2.19	0.43
1:B:1977:LYS:HD3	1:B:1996:LEU:HD22	2.00	0.43
1:B:1138:GLU:OE1	1:B:1138:GLU:N	2.40	0.43
1:B:1601:LEU:O	1:B:1610:LYS:HD3	2.18	0.43
1:B:2103:ASN:HA	1:B:2123:SER:HA	2.01	0.43
1:B:2118:GLN:HB3	1:B:2120:TYR:HE1	1.84	0.43
1:B:1192:PRO:HB2	1:B:1292:PRO:HD3	2.01	0.43
1:B:1749:GLN:H	1:B:1808:MET:HE1	1.84	0.43
1:B:752:LEU:HD11	1:B:780:TYR:HA	2.01	0.43
1:B:709:TYR:CE1	1:B:713:MET:HE3	2.53	0.43
1:B:736[A]:ARG:NH1	1:B:773:GLU:HG2	2.34	0.43
1:B:1364:ILE:HD13	1:B:1424:ILE:HD13	2.01	0.43
1:B:2050:PRO:HA	1:B:2061:GLU:OE2	2.18	0.43
1:B:2103:ASN:HD21	1:B:2121:LYS:HG2	1.84	0.43
1:B:690:VAL:HG11	1:B:707:ILE:HD13	2.01	0.43
1:B:1460:GLY:HA2	1:B:1725:GLU:O	2.19	0.43
1:B:1985:ILE:HD11	1:B:2011:CYS:SG	2.59	0.43
1:B:2000:THR:HB	1:B:2003:GLN:HG3	2.00	0.43
1:B:993:ILE:CD1	1:B:1091:LEU:HD23	2.44	0.42
1:B:1981:SER:O	1:B:1984:ASP:HB2	2.18	0.42
1:B:1262:LEU:HD23	1:B:1262:LEU:HA	1.90	0.42
1:B:1998:GLN:OE1	1:B:1998:GLN:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1953:MET:HG3	1:B:2114:MET:SD	2.60	0.42
1:B:1954:TRP:HB3	1:B:1955:SER:H	1.71	0.42
1:B:971:LYS:HB2	1:B:980:GLN:HB3	2.02	0.42
1:B:1648:ARG:HG3	1:B:1649:SER:N	2.33	0.42
2:J:2090:ILE:HG21	2:J:2111:LEU:HD21	2.01	0.42
2:J:2130:GLY:HA3	2:J:2141:GLU:O	2.20	0.42
1:B:1539:LEU:HD23	1:B:1542:MET:CE	2.48	0.42
1:B:1356:LYS:N	3:B:5803:QB6:O11	2.48	0.42
1:B:1563:VAL:HG12	1:B:1664:MET:HE2	2.02	0.42
1:B:1881:ASN:HD22	1:B:1883:LYS:HZ3	1.66	0.42
2:J:2235:TYR:O	2:J:2239:ARG:HG2	2.20	0.42
1:B:569:LEU:HD13	1:B:596:ILE:CD1	2.50	0.42
1:B:1081:MET:O	1:B:1085:THR:HG23	2.20	0.42
1:B:1961:LYS:HG2	1:B:1971:ILE:HD11	2.01	0.42
1:B:1314:ASN:O	1:B:1318:GLU:HG3	2.19	0.42
1:B:1737:ASN:O	1:B:1741:VAL:HG23	2.20	0.42
1:B:1977:LYS:HD2	1:B:1996:LEU:HD13	2.02	0.42
2:J:2170:LYS:HA	2:J:2170:LYS:HD3	1.87	0.42
1:B:1158:HIS:O	1:B:1171:GLY:HA3	2.20	0.41
1:B:2099:THR:HA	1:B:2126:VAL:HG21	2.02	0.41
1:B:1043:ARG:HB3	2:J:2317:PHE:CE1	2.55	0.41
1:B:1138:GLU:H	1:B:1138:GLU:CD	2.26	0.41
1:B:1448:ILE:O	1:B:1485:ILE:HG12	2.21	0.41
1:B:1931:SER:HA	1:B:2076:LEU:HD13	2.02	0.41
1:B:467:LEU:HD11	1:B:481:LEU:HD21	2.02	0.41
1:B:502:CYS:HA	1:B:652:SER:O	2.20	0.41
1:B:1123:TRP:CD1	1:B:1126:MET:HE1	2.55	0.41
1:B:1356:LYS:HB2	1:B:1356:LYS:HE2	1.94	0.41
1:B:784:ILE:HA	1:B:810:VAL:O	2.21	0.41
1:B:1016:ARG:NH1	5:B:5931:HOH:O	2.53	0.41
1:B:1043:ARG:HB3	2:J:2317:PHE:HE1	1.85	0.41
1:B:2017:ILE:HD13	1:B:2084:LEU:HD23	2.02	0.41
1:B:484:ILE:HG13	1:B:676:PHE:CE2	2.56	0.41
1:B:1223:ILE:O	1:B:1236:HIS:HA	2.21	0.41
1:B:2114:MET:HE2	1:B:2114:MET:HB3	1.92	0.41
2:J:2091:TYR:O	2:J:2224:THR:HA	2.21	0.41
1:B:769:CYS:SG	1:B:774:LEU:HD23	2.61	0.41
1:B:1577:LEU:HD11	1:B:1612:THR:HA	2.02	0.41
1:B:1930:LEU:HD13	1:B:1938:PRO:C	2.46	0.41
1:B:1953:MET:SD	1:B:1962:GLN:HG3	2.61	0.41
1:B:1973:ARG:HG2	1:B:1996:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1477:ILE:O	1:B:1481:ILE:HG12	2.21	0.40
1:B:1269:ARG:NH1	1:B:1279[A]:GLU:OE1	2.55	0.40
1:B:2045:GLU:O	1:B:2046:GLU:HG3	2.21	0.40
1:B:531:ILE:HD12	1:B:531:ILE:N	2.36	0.40
1:B:699:LYS:O	1:B:703:ILE:HG13	2.21	0.40
1:B:705:ASN:HA	1:B:708:VAL:HG12	2.02	0.40
1:B:1043:ARG:HA	1:B:1043:ARG:HD2	1.85	0.40
1:B:1046:ILE:HB	1:B:1064:GLN:NE2	2.35	0.40
1:B:1415:ASP:HB3	1:B:1435:LEU:HD11	2.02	0.40
1:B:1971:ILE:O	1:B:1975:THR:OG1	2.31	0.40
1:B:513:ALA:O	1:B:517:MET:HG3	2.21	0.40
1:B:615:ASP:HA	1:B:651:LEU:HB2	2.04	0.40
1:B:1872:ALA:O	1:B:1875:VAL:HG22	2.21	0.40
1:B:1194:THR:HB	4:B:5810:EDO:H22	2.02	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:696:LYS:NZ	1:B:1695:LEU:O[2_455]	2.08	0.12

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	1726/1747 (99%)	1656 (96%)	64 (4%)	6 (0%)	36	50
2	J	261/263 (99%)	249 (95%)	11 (4%)	1 (0%)	30	43
All	All	1987/2010 (99%)	1905 (96%)	75 (4%)	7 (0%)	30	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	458	GLU
1	B	1859	PRO
1	B	2086	GLN
2	J	2059	PRO
1	B	405	PRO
1	B	528	ASP
1	B	1882	PRO

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	B	1547/1560 (99%)	1459 (94%)	88 (6%)	18	33
2	J	236/236 (100%)	228 (97%)	8 (3%)	32	54
All	All	1783/1796 (99%)	1687 (95%)	96 (5%)	20	35

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	429	GLN
1	B	439	ARG
1	B	457	SER
1	B	465	GLU
1	B	469	LYS
1	B	481	LEU
1	B	484	ILE
1	B	489	TYR
1	B	490	ARG
1	B	495	THR
1	B	510	THR
1	B	525	ILE
1	B	530	THR
1	B	545	ARG
1	B	551	MET
1	B	554	SER
1	B	607	GLN

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Mol	Chain	Res	Type
1	B	696	LYS
1	B	699	LYS
1	B	734	THR
1	B	743	LEU
1	B	759	THR
1	B	760	GLU
1	B	797	VAL
1	B	847	LEU
1	B	893	MET
1	B	984	LEU
1	B	1009	LEU
1	B	1032	GLU
1	B	1044	VAL
1	B	1051	SER
1	B	1054	GLU
1	B	1072	LEU
1	B	1073	GLU
1	B	1113	ASN
1	B	1126	MET
1	B	1137	GLU
1	B	1141	LYS
1	B	1147	ASN
1	B	1187	SER
1	B	1212	GLU
1	B	1284	VAL
1	B	1310	SER
1	B	1322	GLN
1	B	1342	SER
1	B	1346	VAL
1	B	1357	THR
1	B	1391	MET
1	B	1414	THR
1	B	1507	SER
1	B	1585	GLN
1	B	1596	ASP
1	B	1597	LEU
1	B	1598	ILE
1	B	1603	LYS
1	B	1625	SER
1	B	1731	CYS
1	B	1732	MET
1	B	1742	THR

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Mol	Chain	Res	Type
1	B	1772	ASN
1	B	1781	LEU
1	B	1788	LEU
1	B	1791	GLN
1	B	1831	LEU
1	B	1847	GLU
1	B	1848	ILE
1	B	1856	GLU
1	B	1858	ILE
1	B	1860	ILE
1	B	1877	HIS
1	B	1904	LEU
1	B	1907	GLU
1	B	1929	VAL
1	B	1945	LEU
1	B	1958	SER
1	B	1967	THR
1	B	1980	GLU
1	B	1985	ILE
1	B	1990	ASP
1	B	1998	GLN
1	B	2000	THR
1	B	2029	ILE
1	B	2059	LYS
1	B	2062	GLU
1	B	2067	VAL
1	B	2073	SER
1	B	2082	LEU
1	B	2095	VAL
2	J	2076	ARG
2	J	2095	ASP
2	J	2170	LYS
2	J	2171	GLU
2	J	2219	THR
2	J	2226	THR
2	J	2233	SER
2	J	2239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	805	HIS

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Mol	Chain	Res	Type
1	B	877	GLN
1	B	892	GLN
1	B	980	GLN
1	B	1113	ASN
1	B	1158	HIS
1	B	1305	GLN
1	B	1370	GLN
1	B	1531	ASN
1	B	1553	HIS
1	B	1591	HIS
1	B	1696	GLN
1	B	1730	HIS
1	B	1772	ASN
1	B	1798	GLN
1	B	1881	ASN
1	B	1947	GLN
1	B	1994	ASN
1	B	2118	GLN
2	J	2084	HIS
2	J	2089	HIS
2	J	2158	HIS
2	J	2241	ASN
2	J	2255	HIS

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](#)

20 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	5810	-	3,3,3	0.55	0	2,2,2	0.51	0
4	EDO	B	5814	-	3,3,3	0.78	0	2,2,2	0.30	0
4	EDO	B	5811	-	3,3,3	0.64	0	2,2,2	0.32	0
4	EDO	B	5812	-	3,3,3	0.47	0	2,2,2	0.43	0
4	EDO	B	5805	-	3,3,3	0.34	0	2,2,2	0.96	0
4	EDO	J	2401	-	3,3,3	0.46	0	2,2,2	0.45	0
3	QB6	B	5802	-	12,12,12	2.31	6 (50%)	18,18,18	2.57	5 (27%)
4	EDO	B	5807	-	3,3,3	0.67	0	2,2,2	0.34	0
4	EDO	B	5804	-	3,3,3	0.31	0	2,2,2	1.05	0
4	EDO	B	5816	-	3,3,3	0.65	0	2,2,2	0.38	0
4	EDO	B	5815	-	3,3,3	0.37	0	2,2,2	0.94	0
3	QB6	J	2402	-	12,12,12	2.50	5 (41%)	18,18,18	3.29	6 (33%)
4	EDO	B	5817	-	3,3,3	0.57	0	2,2,2	0.40	0
4	EDO	B	5813	-	3,3,3	0.49	0	2,2,2	0.68	0
4	EDO	B	5809	-	3,3,3	0.48	0	2,2,2	0.47	0
4	EDO	B	5808	-	3,3,3	0.48	0	2,2,2	0.42	0
4	EDO	J	2403	-	3,3,3	0.55	0	2,2,2	0.14	0
4	EDO	B	5806	-	3,3,3	0.38	0	2,2,2	1.43	0
3	QB6	B	5801	-	12,12,12	2.48	6 (50%)	18,18,18	2.78	4 (22%)
3	QB6	B	5803	-	12,12,12	2.57	4 (33%)	18,18,18	4.80	8 (44%)

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	5810	-	-	0/1/1/1	-
4	EDO	B	5814	-	-	1/1/1/1	-
4	EDO	B	5811	-	-	1/1/1/1	-
4	EDO	B	5812	-	-	0/1/1/1	-
4	EDO	B	5805	-	-	0/1/1/1	-
4	EDO	J	2401	-	-	1/1/1/1	-
3	QB6	B	5802	-	-	4/6/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	5807	-	-	1/1/1/1	-
4	EDO	B	5804	-	-	1/1/1/1	-
4	EDO	B	5816	-	-	0/1/1/1	-
4	EDO	B	5815	-	-	1/1/1/1	-
3	QB6	J	2402	-	-	4/6/6/6	0/1/1/1
4	EDO	B	5817	-	-	1/1/1/1	-
4	EDO	B	5813	-	-	1/1/1/1	-
4	EDO	B	5809	-	-	0/1/1/1	-
4	EDO	B	5808	-	-	1/1/1/1	-
4	EDO	J	2403	-	-	1/1/1/1	-
4	EDO	B	5806	-	-	1/1/1/1	-
3	QB6	B	5801	-	-	4/6/6/6	0/1/1/1
3	QB6	B	5803	-	-	4/6/6/6	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2402	QB6	S09-N10	5.90	1.71	1.60
3	B	5803	QB6	S09-N10	5.89	1.71	1.60
3	B	5801	QB6	S09-N10	5.79	1.71	1.60
3	B	5802	QB6	S09-N10	5.58	1.71	1.60
3	B	5803	QB6	C07-S09	5.00	1.84	1.77
3	B	5801	QB6	C07-S09	3.93	1.83	1.77
3	J	2402	QB6	C07-S09	3.84	1.83	1.77
3	B	5802	QB6	C07-S09	2.96	1.81	1.77
3	B	5801	QB6	O12-S09	2.93	1.48	1.43
3	B	5803	QB6	O04-C03	2.83	1.42	1.36
3	J	2402	QB6	C02-N01	2.75	1.47	1.38
3	J	2402	QB6	O12-S09	2.64	1.48	1.43
3	B	5803	QB6	C02-N01	2.58	1.46	1.38
3	J	2402	QB6	O04-C03	2.51	1.41	1.36
3	B	5802	QB6	O11-S09	2.45	1.48	1.43
3	B	5802	QB6	C02-N01	2.45	1.46	1.38
3	B	5802	QB6	O12-S09	2.38	1.47	1.43
3	B	5801	QB6	O04-C03	2.31	1.41	1.36
3	B	5802	QB6	O04-C03	2.22	1.40	1.36
3	B	5801	QB6	C02-N01	2.19	1.45	1.38
3	B	5801	QB6	O11-S09	2.05	1.47	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5803	QB6	O12-S09-O11	-15.13	95.53	118.80
3	J	2402	QB6	O12-S09-O11	-11.89	100.51	118.80
3	B	5803	QB6	O12-S09-C07	10.87	119.63	107.35
3	B	5801	QB6	O12-S09-O11	-10.03	103.38	118.80
3	B	5802	QB6	O12-S09-O11	-8.76	105.33	118.80
3	B	5803	QB6	O12-S09-N10	4.22	113.44	107.35
3	J	2402	QB6	O11-S09-C07	4.00	111.87	107.35
3	J	2402	QB6	O12-S09-N10	3.67	112.64	107.35
3	B	5803	QB6	O04-C03-C02	3.59	122.39	116.50
3	B	5802	QB6	C07-S09-N10	3.47	113.23	108.40
3	B	5801	QB6	O11-S09-N10	3.42	112.29	107.35
3	B	5803	QB6	C08-C07-S09	3.15	125.02	119.34
3	B	5803	QB6	C05-C06-C07	2.98	122.34	119.44
3	J	2402	QB6	C07-S09-N10	2.93	112.48	108.40
3	B	5801	QB6	O12-S09-C07	2.83	110.55	107.35
3	B	5802	QB6	C03-C02-N01	2.71	122.78	118.59
3	B	5802	QB6	O04-C03-C02	2.64	120.83	116.50
3	J	2402	QB6	O04-C03-C02	2.46	120.54	116.50
3	J	2402	QB6	O11-S09-N10	2.44	110.87	107.35
3	B	5801	QB6	O12-S09-N10	2.40	110.81	107.35
3	B	5803	QB6	C06-C07-S09	-2.30	116.60	119.72
3	B	5802	QB6	O12-S09-N10	2.16	110.46	107.35
3	B	5803	QB6	O11-S09-N10	2.07	110.33	107.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	5806	EDO	O1-C1-C2-O2
4	B	5807	EDO	O1-C1-C2-O2
4	B	5811	EDO	O1-C1-C2-O2
3	B	5802	QB6	C06-C07-S09-N10
3	B	5801	QB6	C06-C07-S09-O12
3	B	5802	QB6	C08-C07-S09-N10
3	B	5803	QB6	C08-C07-S09-N10
3	B	5801	QB6	C08-C07-S09-N10
3	B	5803	QB6	C06-C07-S09-N10
3	B	5801	QB6	C08-C07-S09-O12
3	J	2402	QB6	C08-C07-S09-N10
4	B	5815	EDO	O1-C1-C2-O2
4	B	5817	EDO	O1-C1-C2-O2
3	J	2402	QB6	C06-C07-S09-N10
3	B	5801	QB6	C06-C07-S09-N10

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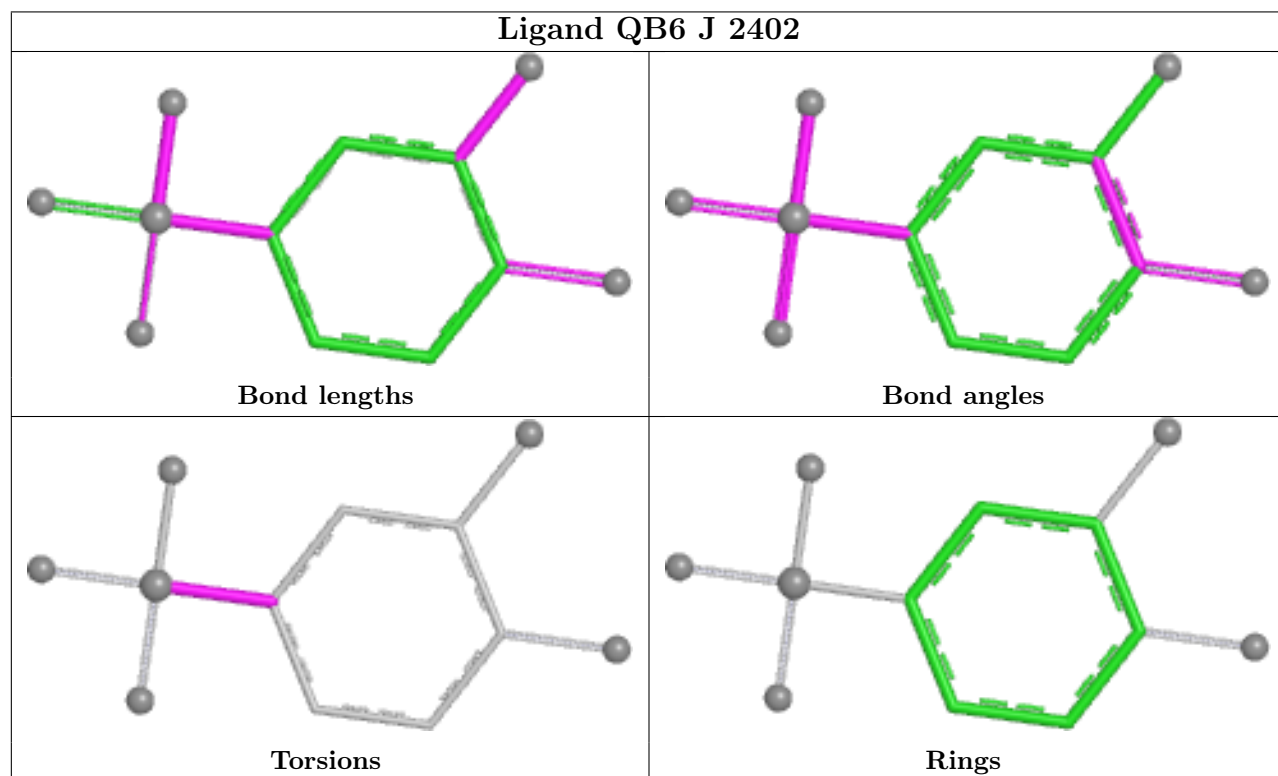
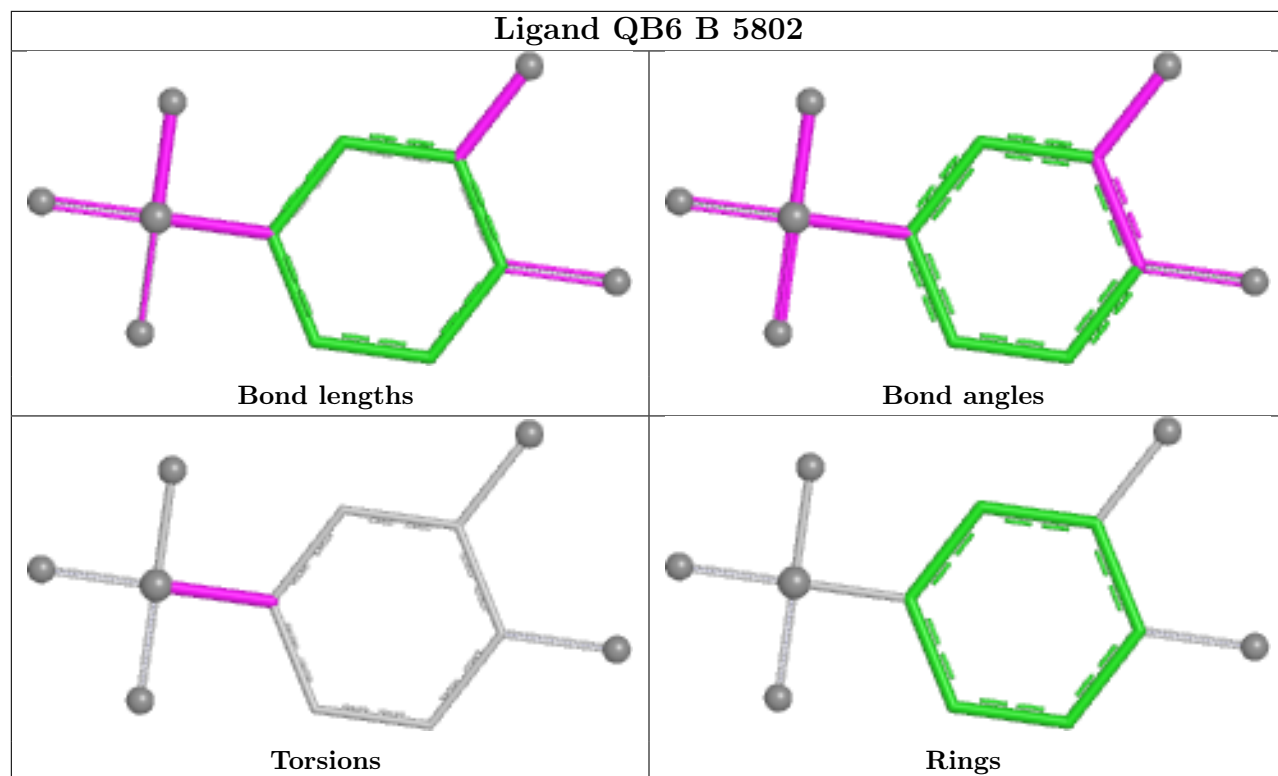
Mol	Chain	Res	Type	Atoms
4	J	2403	EDO	O1-C1-C2-O2
3	B	5803	QB6	C06-C07-S09-O11
4	B	5808	EDO	O1-C1-C2-O2
3	B	5803	QB6	C08-C07-S09-O11
3	J	2402	QB6	C08-C07-S09-O11
4	B	5804	EDO	O1-C1-C2-O2
4	J	2401	EDO	O1-C1-C2-O2
3	B	5802	QB6	C06-C07-S09-O11
3	J	2402	QB6	C06-C07-S09-O11
3	B	5802	QB6	C08-C07-S09-O11
4	B	5813	EDO	O1-C1-C2-O2
4	B	5814	EDO	O1-C1-C2-O2

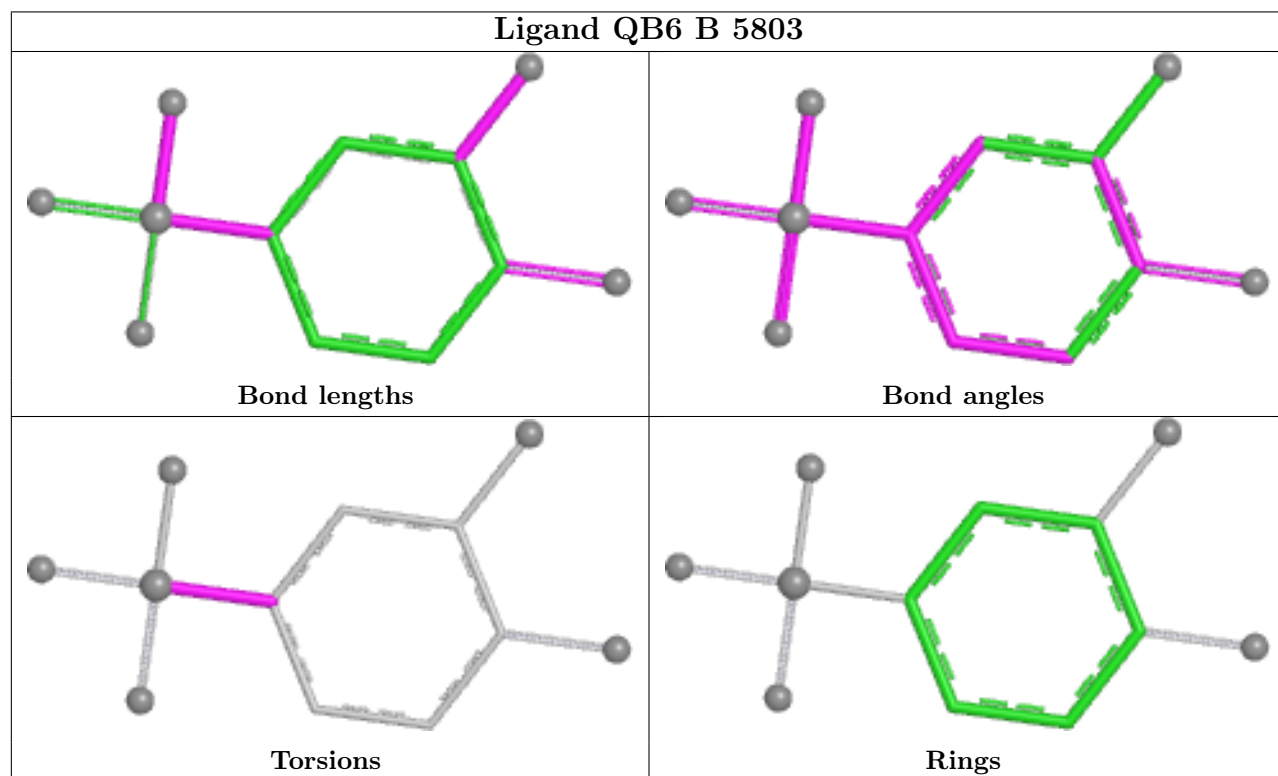
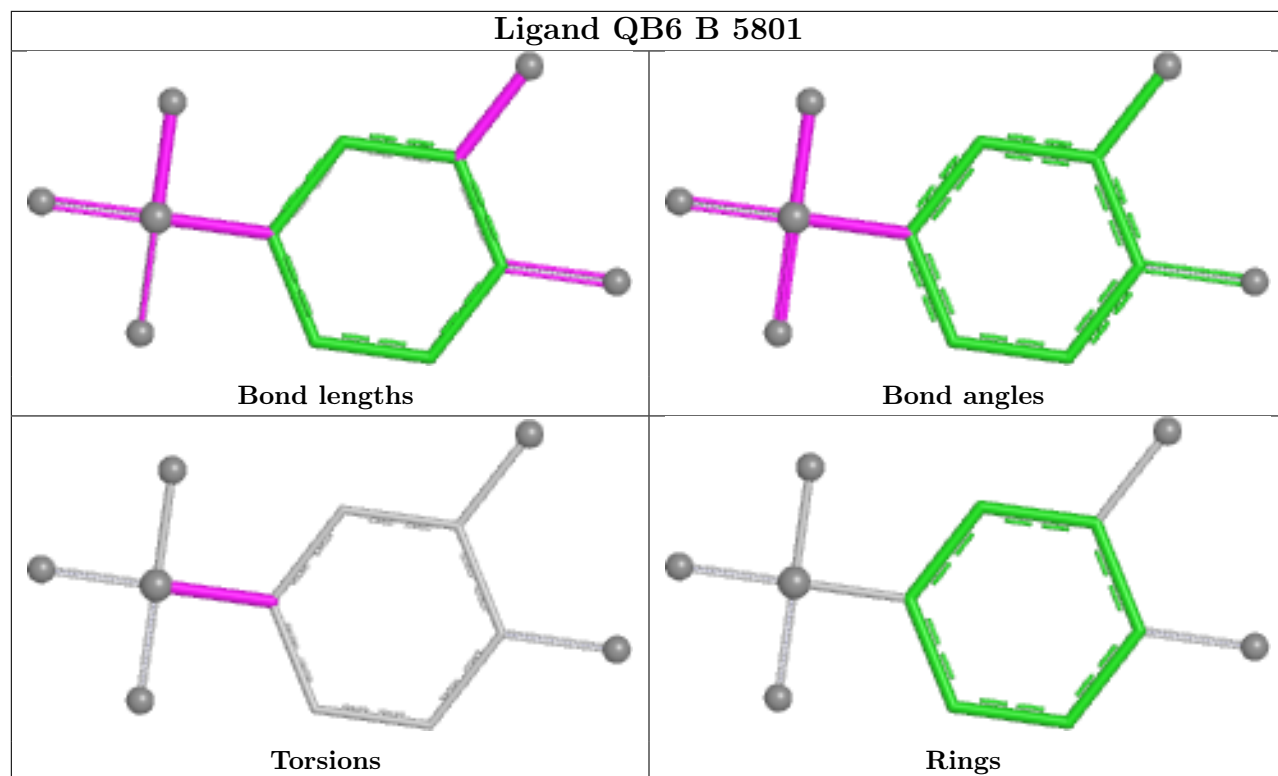
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5810	EDO	2	0
4	B	5804	EDO	2	0
4	B	5816	EDO	2	0
4	B	5813	EDO	1	0
4	J	2403	EDO	1	0
3	B	5803	QB6	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	B	1724/1747 (98%)	0.64	130 (7%)	20 17	25, 66, 142, 226	4 (0%)
2	J	263/263 (100%)	0.51	14 (5%)	32 28	36, 59, 122, 203	0
All	All	1987/2010 (98%)	0.62	144 (7%)	21 18	25, 65, 140, 226	4 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1858	ILE	5.8
1	B	1601	LEU	4.7
1	B	1604	LEU	4.6
2	J	2060	LEU	4.6
1	B	454	PRO	4.5
2	J	2058	GLY	4.5
1	B	404	ALA	4.3
1	B	1501	ALA	4.3
1	B	1936	LEU	4.2
1	B	2124	VAL	4.2
1	B	456	GLY	4.0
1	B	575	LEU	4.0
1	B	1890	LYS	3.9
1	B	455	PHE	3.8
1	B	1871	LEU	3.8
1	B	1584	ILE	3.7
1	B	1940	LEU	3.7
1	B	1307	LEU	3.6
1	B	2037	VAL	3.6
1	B	1958	SER	3.6
1	B	2024	VAL	3.6
1	B	1868	LEU	3.5
1	B	1996	LEU	3.5
1	B	2036	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1360	ALA	3.4
1	B	1904	LEU	3.3
1	B	726	HIS	3.3
2	J	2097	ILE	3.3
2	J	2318	ALA	3.2
1	B	1971	ILE	3.2
1	B	1954	TRP	3.2
1	B	1044	VAL	3.1
1	B	1860	ILE	3.1
1	B	1899	LEU	3.1
1	B	1943	MET	3.1
1	B	1174	ILE	3.0
1	B	1876	PRO	3.0
1	B	782	PHE	2.9
1	B	1997	LEU	2.9
1	B	1849	ILE	2.9
1	B	2120	TYR	2.9
1	B	1864	GLU	2.9
1	B	1931	SER	2.8
1	B	1982	VAL	2.8
1	B	1597	LEU	2.8
1	B	1321	TYR	2.8
1	B	1879	LEU	2.8
2	J	2319	LEU	2.7
1	B	2010	PHE	2.7
2	J	2061	GLY	2.7
1	B	1877	HIS	2.7
1	B	1140	VAL	2.7
1	B	604	THR	2.7
1	B	1852	ALA	2.6
1	B	2105	THR	2.6
1	B	1143	ILE	2.6
1	B	1908	LEU	2.6
1	B	1336	PHE	2.6
1	B	1308	PRO	2.6
1	B	1865	ASP	2.6
1	B	2056	PHE	2.6
1	B	1355	GLY	2.6
1	B	2107	TYR	2.6
1	B	1573	ALA	2.6
1	B	2035	VAL	2.6
1	B	1922	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	582	ALA	2.5
1	B	1222	TRP	2.5
1	B	570	THR	2.5
1	B	1164	LEU	2.5
1	B	1880	ASN	2.5
1	B	1919	ALA	2.5
1	B	452	PRO	2.5
1	B	2097	PRO	2.5
2	J	2317	PHE	2.4
1	B	1963	LEU	2.4
1	B	2038	LEU	2.4
2	J	2320	LEU	2.4
1	B	805	HIS	2.4
1	B	2112	ALA	2.4
1	B	601	GLY	2.4
2	J	2062	SER	2.4
1	B	1451	PHE	2.4
1	B	1748	LYS	2.4
1	B	1382	MET	2.4
1	B	2066	VAL	2.4
1	B	639	ILE	2.4
1	B	1688	VAL	2.4
2	J	2063	MET	2.4
1	B	1956	LYS	2.3
1	B	1788	LEU	2.3
1	B	420	SER	2.3
1	B	1514	PHE	2.3
1	B	1598	ILE	2.3
1	B	752	LEU	2.2
1	B	1041	LEU	2.2
1	B	1789	VAL	2.3
1	B	2040	GLN	2.2
1	B	935	LEU	2.2
1	B	1148	PHE	2.2
1	B	528	ASP	2.2
1	B	405	PRO	2.2
1	B	574	GLN	2.2
1	B	1848	ILE	2.2
1	B	1845	LEU	2.2
1	B	2034	PRO	2.2
2	J	2285	GLY	2.2
1	B	1863	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	457	SER	2.2
1	B	1317	PHE	2.2
1	B	1512	PHE	2.2
1	B	1859	PRO	2.2
1	B	821	LEU	2.1
1	B	1419	LEU	2.1
1	B	1895	LEU	2.1
1	B	1505	GLY	2.1
1	B	2113	TYR	2.1
1	B	1660	LEU	2.1
1	B	1894	LEU	2.1
1	B	1149	PRO	2.1
2	J	2092	VAL	2.1
1	B	1328	PHE	2.1
1	B	1893	LEU	2.1
1	B	2076	LEU	2.1
2	J	2090	ILE	2.1
1	B	603	ARG	2.1
1	B	716	ALA	2.1
1	B	1603	LYS	2.1
1	B	1853	ALA	2.1
1	B	2096	ALA	2.1
1	B	641	MET	2.1
1	B	1862	HIS	2.1
1	B	1600	TYR	2.1
1	B	2090	VAL	2.1
1	B	1884	PHE	2.1
1	B	2091	LYS	2.0
1	B	1906	ALA	2.0
1	B	424	ALA	2.0
1	B	943	LEU	2.0
1	B	1072	LEU	2.0
1	B	1916	LEU	2.0
1	B	2092	LEU	2.0
1	B	1052	ILE	2.0
2	J	2098	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

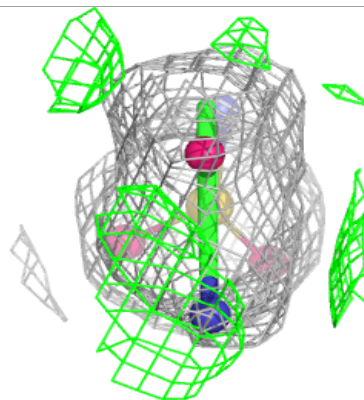
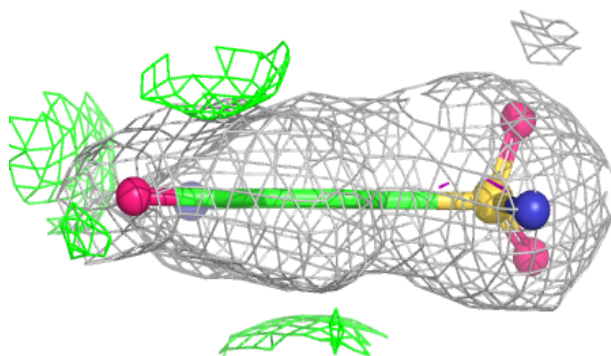
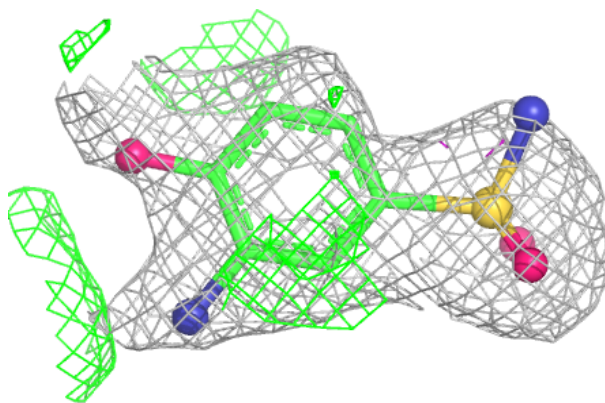
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	EDO	B	5810	4/4	0.76	0.15	53,59,60,60	0
4	EDO	B	5814	4/4	0.76	0.23	41,46,51,56	0
4	EDO	B	5809	4/4	0.78	0.15	57,60,62,67	0
4	EDO	B	5816	4/4	0.79	0.16	44,58,60,67	0
4	EDO	B	5817	4/4	0.79	0.17	56,58,58,61	0
4	EDO	J	2401	4/4	0.79	0.14	66,70,72,79	0
4	EDO	B	5815	4/4	0.82	0.17	51,52,66,66	0
3	QB6	B	5803	12/12	0.82	0.17	56,67,74,74	0
4	EDO	B	5813	4/4	0.84	0.14	42,46,51,51	0
4	EDO	B	5807	4/4	0.85	0.21	42,46,54,55	0
4	EDO	B	5804	4/4	0.87	0.13	46,52,61,72	0
3	QB6	J	2402	12/12	0.88	0.10	60,65,68,74	0
3	QB6	B	5802	12/12	0.88	0.11	62,69,74,76	0
4	EDO	B	5806	4/4	0.88	0.12	39,41,42,48	0
4	EDO	J	2403	4/4	0.88	0.14	47,48,54,58	0
4	EDO	B	5811	4/4	0.89	0.10	54,54,55,57	0
4	EDO	B	5808	4/4	0.89	0.12	61,63,65,70	0
4	EDO	B	5812	4/4	0.92	0.12	60,63,63,69	0
3	QB6	B	5801	12/12	0.93	0.09	48,54,58,60	0
4	EDO	B	5805	4/4	0.93	0.12	43,48,50,65	0

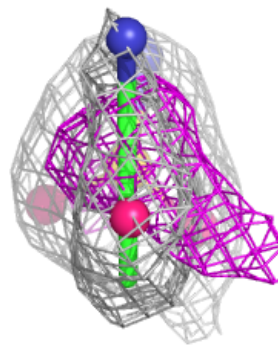
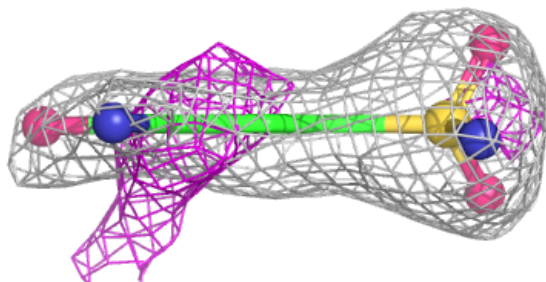
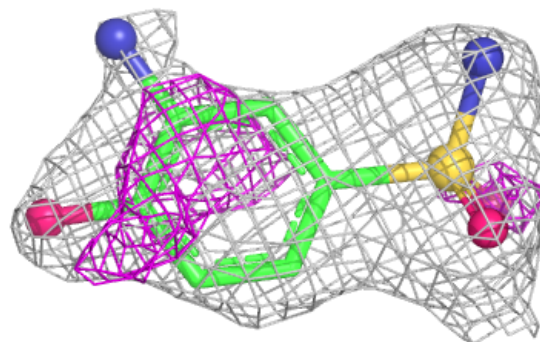
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QB6 B 5803:

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

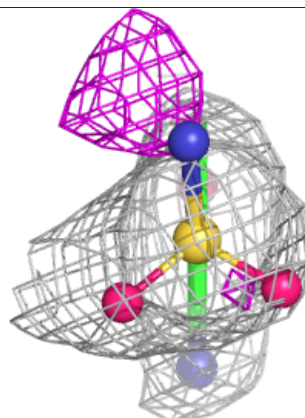
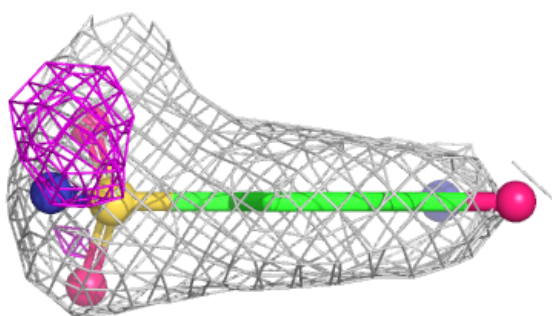
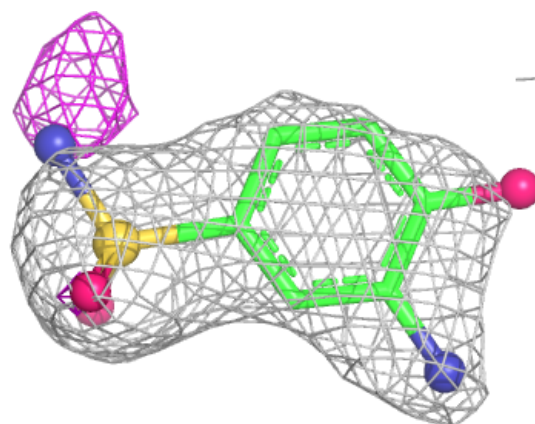
**Electron density around QB6 J 2402:**

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

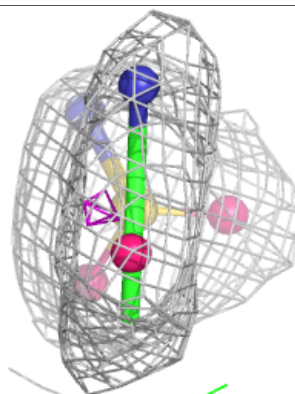
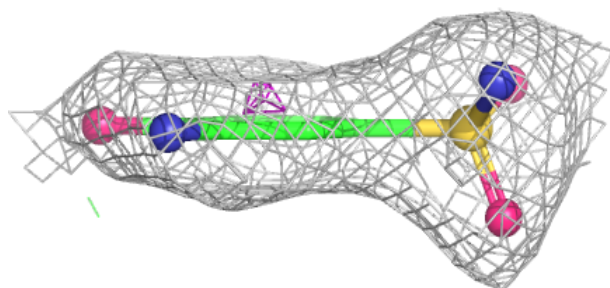
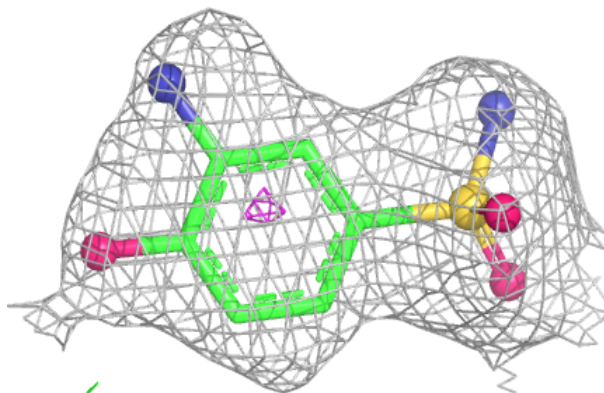


Electron density around QB6 B 5802:

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

**Electron density around QB6 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.