



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:08 AM UTC

PDB ID : 8BCE / pdb_00008bce
Title : Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and compound 76
Authors : Vester, K.; Loll, B.; Wahl, M.C.
Deposited on : 2022-10-15
Resolution : 2.05 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

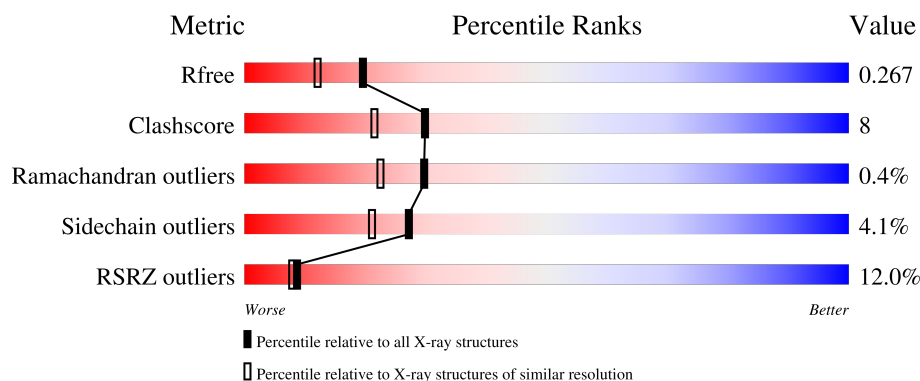
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	13% 76% 20% ..
2	J	263	6% 85% 14%

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
4	EDO	B	5811	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16532 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
1	B	1719	Total	C	N	O	S	0	0	0
			13822	8833	2366	2551	72			

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

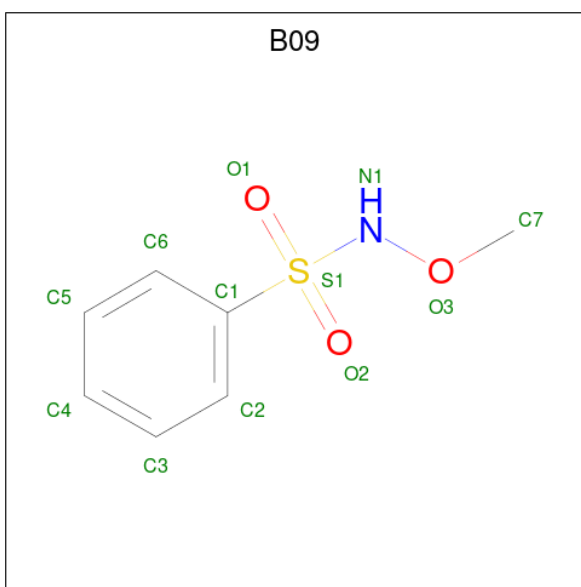
- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

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

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 N-methoxybenzenesulfonamide (CCD ID: B09) (formula: C₇H₉NO₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			12	7	1	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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		

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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	J	1	Total C O 4 2 2	0	0

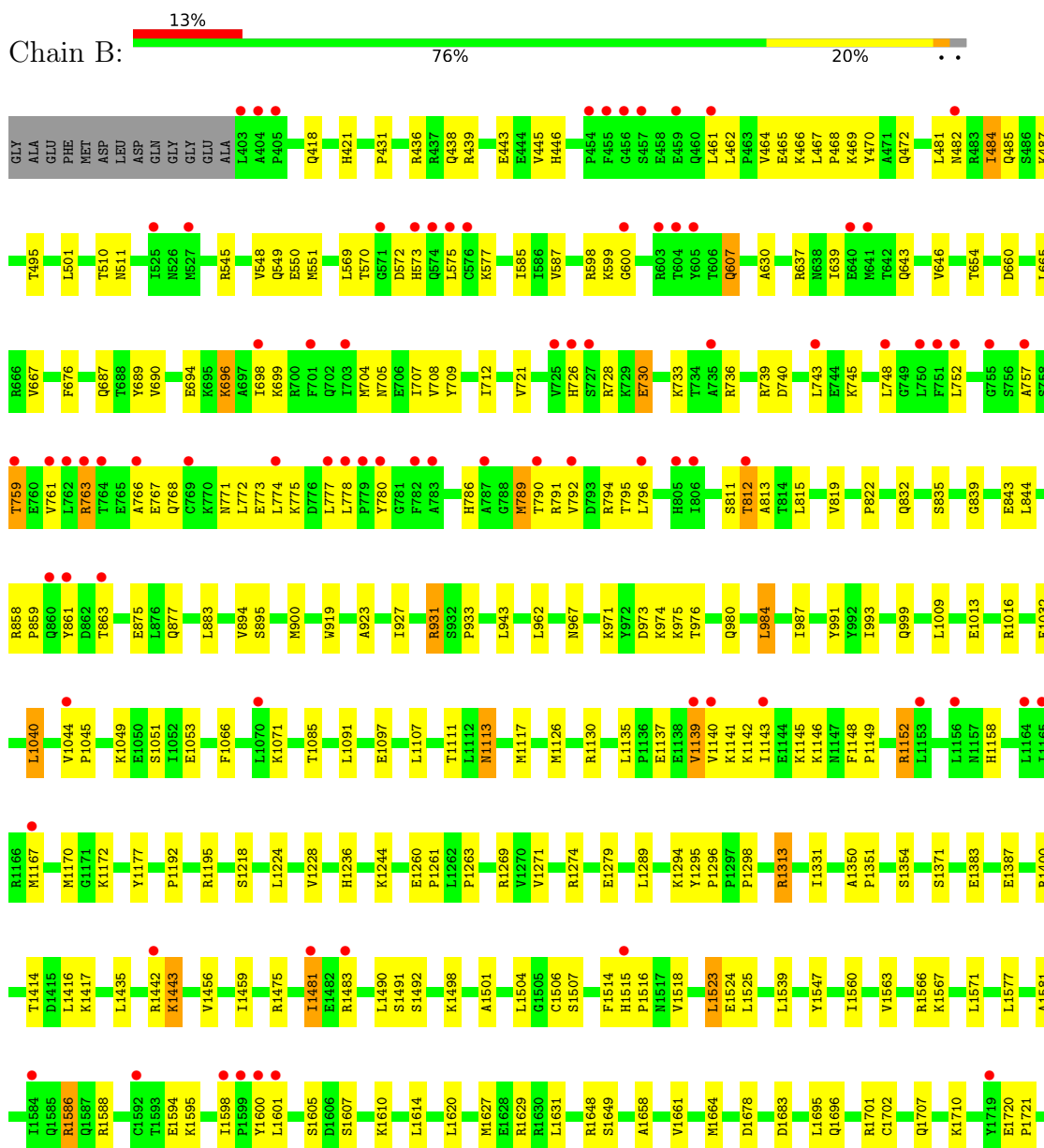
- Molecule 5 is water.

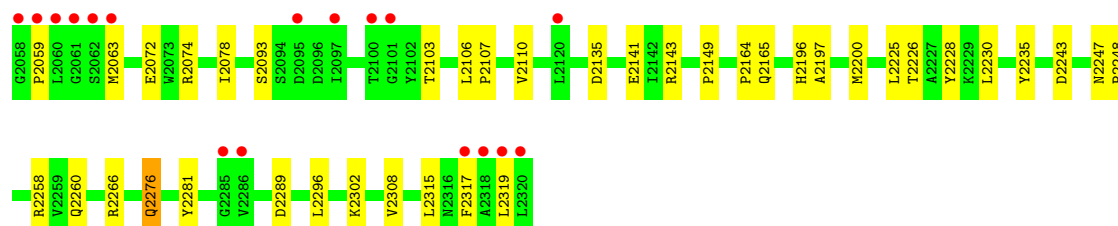
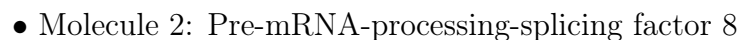
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	449	Total O 449 449	0	2
5	J	78	Total O 78 78	0	0

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.05Å 119.05Å 188.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.51 – 2.05 48.51 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.51-2.05) 98.9 (48.51-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.220 , 0.267 0.221 , 0.267	Depositor DCC
R_{free} test set	2096 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16532	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: B09, 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	0.40	0/14115	0.59	0/19125
2	J	0.43	0/2190	0.61	0/2981
All	All	0.40	0/16305	0.59	0/22106

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	13822	0	13969	253	0
2	J	2123	0	2063	22	0
3	B	12	0	9	0	0
4	B	44	0	66	7	0
4	J	4	0	6	0	0
5	B	449	0	0	11	0
5	J	78	0	0	2	0
All	All	16532	0	16113	272	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 8.

All (272) 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)
2:J:2276:GLN:OE1	5:J:2501:HOH:O	1.94	0.86
1:B:1861:ARG:HH21	1:B:1863:HIS:HB2	1.43	0.82
1:B:763:ARG:HH21	1:B:767:GLU:HG3	1.44	0.81
1:B:993:ILE:HD12	1:B:1091:LEU:HD23	1.64	0.80
1:B:1860:ILE:HD12	1:B:1861:ARG:HG2	1.66	0.76
1:B:421:HIS:NE2	1:B:875:GLU:OE1	2.19	0.76
1:B:1296:PRO:HG2	1:B:1498:LYS:HE3	1.67	0.75
1:B:1707:GLN:HG2	4:B:5802:EDO:H21	1.69	0.75
2:J:2103:THR:HG23	2:J:2260:GLN:HG2	1.69	0.74
1:B:2043:ARG:NH2	1:B:2084:LEU:O	2.19	0.74
1:B:2006:ASP:OD1	1:B:2009:ARG:NH1	2.19	0.72
1:B:1843:ARG:HD2	1:B:1877:HIS:HA	1.71	0.72
1:B:739:ARG:NH1	1:B:740:ASP:OD1	2.23	0.72
1:B:771:ASN:HB3	1:B:774:LEU:HB2	1.70	0.72
2:J:2200:MET:HE1	2:J:2230:LEU:HD12	1.70	0.71
1:B:1747:ASN:HB2	1:B:1808:MET:HE3	1.74	0.69
1:B:572:ASP:OD2	1:B:1274:ARG:NH1	2.26	0.69
2:J:2093:SER:OG	2:J:2226:THR:HG22	1.95	0.67
1:B:2000:THR:HB	1:B:2003:GLN:HG3	1.77	0.67
1:B:2032:GLY:N	1:B:2096:ALA:O	2.27	0.66
1:B:1142:LYS:NZ	1:B:1167:MET:SD	2.69	0.66
1:B:654:THR:HG21	1:B:676:PHE:O	1.94	0.66
1:B:1814:ASN:HA	1:B:1817:MET:HE3	1.77	0.66
1:B:2015:PRO:HG2	1:B:2116:CYS:SG	2.35	0.66
2:J:2141:GLU:OE2	2:J:2266:ARG:NH2	2.28	0.66
1:B:1271:VAL:HG22	1:B:1279:GLU:HG3	1.78	0.65
1:B:1298:PRO:HB3	1:B:1515:HIS:CG	2.32	0.65
1:B:1914:GLU:O	1:B:1917:SER:HB2	1.95	0.65
1:B:698:ILE:HD12	1:B:698:ILE:H	1.61	0.64
1:B:2038:LEU:HD21	1:B:2089:LYS:HG3	1.79	0.64
1:B:1594:GLU:OE1	1:B:1594:GLU:N	2.23	0.63
1:B:1158:HIS:HD2	1:B:1172:LYS:HA	1.63	0.62
1:B:436:ARG:HG3	1:B:445:VAL:HG22	1.81	0.62
1:B:1475:ARG:HD2	1:B:1504:LEU:HA	1.79	0.62
1:B:748:LEU:HD11	1:B:780:TYR:HB3	1.82	0.62
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	1.81	0.62
1:B:1195:ARG:H	4:B:5811:EDO:H12	1.65	0.61
1:B:2078:SER:OG	1:B:2093:ASP:O	2.17	0.61
2:J:2141:GLU:OE1	2:J:2143:ARG:NH2	2.32	0.61
1:B:789:MET:O	1:B:794:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2078:SER:HB3	1:B:2092:LEU:HD22	1.83	0.60
1:B:1130:ARG:HG3	1:B:1140:VAL:HG11	1.81	0.60
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.82	0.60
1:B:1620:LEU:HD22	1:B:1629:ARG:HG2	1.82	0.60
1:B:630:ALA:HB2	1:B:900:MET:HE3	1.83	0.60
1:B:1443:LYS:H	1:B:1443:LYS:HD2	1.67	0.60
1:B:991:TYR:OH	1:B:1097:GLU:OE1	2.13	0.59
1:B:1524:GLU:OE1	5:B:5901:HOH:O	2.16	0.59
1:B:1547:TYR:OH	1:B:1588:ARG:NH2	2.35	0.59
1:B:774:LEU:O	1:B:778:LEU:HB2	2.02	0.59
1:B:962:LEU:HD21	1:B:974:LYS:HE3	1.84	0.59
1:B:570:THR:HG22	1:B:572:ASP:H	1.67	0.59
1:B:1903:GLN:NE2	1:B:1904:LEU:O	2.27	0.58
1:B:660:ASP:OD1	1:B:931:ARG:HD3	2.03	0.57
1:B:1113:ASN:O	1:B:1117:MET:HG3	2.03	0.57
1:B:1891:THR:HA	1:B:1894:LEU:HB3	1.85	0.57
1:B:811:SER:OG	1:B:812:THR:N	2.38	0.57
1:B:1861:ARG:CZ	1:B:1864:GLU:HG2	2.35	0.57
1:B:2019:LEU:HD23	1:B:2019:LEU:H	1.69	0.57
1:B:984:LEU:HD23	5:B:6268:HOH:O	2.05	0.56
1:B:1049:LYS:O	1:B:1049:LYS:HD3	2.05	0.56
2:J:2106:LEU:HD12	2:J:2107:PRO:HD2	1.86	0.56
1:B:1498:LYS:HE2	1:B:1498:LYS:H	1.71	0.55
1:B:812:THR:OG1	1:B:813:ALA:N	2.39	0.55
1:B:1886:ASP:HB2	1:B:1889:VAL:HB	1.88	0.55
1:B:1294:LYS:HA	4:B:5811:EDO:H21	1.88	0.55
1:B:1498:LYS:H	1:B:1498:LYS:CE	2.20	0.55
1:B:2006:ASP:HA	1:B:2009:ARG:NH1	2.23	0.54
1:B:894:VAL:HG22	5:B:6034:HOH:O	2.07	0.54
1:B:1501:ALA:HB1	1:B:1506:CYS:HB2	1.89	0.54
1:B:1456:VAL:HG12	1:B:1491:SER:HB2	1.89	0.54
1:B:1236:HIS:ND1	5:B:5905:HOH:O	2.34	0.54
1:B:1867:LEU:O	1:B:1871:LEU:HG	2.08	0.54
1:B:1953:MET:C	1:B:1954:TRP:HD1	2.16	0.54
1:B:2019:LEU:HD22	1:B:2118:GLN:HE22	1.73	0.54
1:B:1974:CYS:HB3	1:B:1979:VAL:HG23	1.90	0.54
1:B:2021:TYR:OH	1:B:2121:LYS:O	2.27	0.53
1:B:973:ASP:OD1	1:B:975:LYS:HG2	2.09	0.53
1:B:1908:LEU:H	1:B:1908:LEU:HD22	1.73	0.53
2:J:2266:ARG:NE	5:J:2502:HOH:O	2.39	0.53
1:B:1865:ASP:OD1	1:B:1884:PHE:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLN:NE2	5:B:5915:HOH:O	2.41	0.53
1:B:2068:ILE:HG22	1:B:2092:LEU:HD13	1.90	0.53
1:B:1581:ALA:HA	1:B:1586:ARG:HG2	1.90	0.53
1:B:709:TYR:OH	1:B:745:LYS:HD3	2.09	0.52
1:B:2066:VAL:HG12	1:B:2092:LEU:HD11	1.92	0.52
1:B:822:PRO:HG2	1:B:858:ARG:HG2	1.90	0.52
1:B:1953:MET:SD	1:B:1962:GLN:HG3	2.50	0.52
1:B:599:LYS:NZ	5:B:5916:HOH:O	2.42	0.52
1:B:748:LEU:HD21	1:B:780:TYR:HD1	1.75	0.52
2:J:2196:HIS:HD2	2:J:2200:MET:HE2	1.75	0.52
1:B:1648:ARG:HG3	1:B:1649:SER:N	2.23	0.52
1:B:858:ARG:HE	1:B:861:TYR:HD2	1.58	0.52
1:B:1442:ARG:HA	1:B:1442:ARG:HH11	1.75	0.51
1:B:1871:LEU:O	1:B:1875:VAL:HG13	2.11	0.51
1:B:1846:ILE:HG23	1:B:1895:LEU:HD12	1.93	0.51
1:B:1224:LEU:HD23	1:B:1236:HIS:HB2	1.91	0.51
1:B:1107:LEU:O	1:B:1111:THR:HG23	2.09	0.51
2:J:2197:ALA:HA	2:J:2200:MET:HE3	1.92	0.51
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.46	0.51
1:B:1313:ARG:NH1	5:B:5919:HOH:O	2.44	0.51
1:B:1822:TYR:O	1:B:1921:ARG:HD2	2.10	0.51
1:B:1967:THR:HG22	1:B:1970:HIS:CE1	2.46	0.51
1:B:1804:ILE:HG12	1:B:1810:VAL:HG12	1.93	0.50
1:B:2068:ILE:O	1:B:2077:ILE:HG13	2.11	0.50
1:B:485:GLN:HE21	1:B:511:ASN:HB2	1.77	0.50
1:B:923:ALA:O	1:B:927:ILE:HD12	2.10	0.50
1:B:1953:MET:HE2	1:B:2114:MET:HE3	1.93	0.50
1:B:461:LEU:HD12	1:B:481:LEU:O	2.12	0.50
1:B:726:HIS:CE1	1:B:844:LEU:HD11	2.47	0.50
1:B:484:ILE:HD11	1:B:501:LEU:HD21	1.93	0.50
1:B:598:ARG:HH22	4:B:5809:EDO:C2	2.24	0.50
1:B:2041:LEU:O	1:B:2087:LYS:HA	2.12	0.50
1:B:690:VAL:HG11	1:B:707:ILE:HD13	1.93	0.49
1:B:835:SER:O	1:B:839:GLY:N	2.45	0.49
1:B:1195:ARG:N	4:B:5811:EDO:H12	2.27	0.49
1:B:1139:VAL:O	1:B:1143:ILE:HG13	2.13	0.49
1:B:1861:ARG:HH21	1:B:1863:HIS:CB	2.21	0.49
1:B:2037:VAL:HG13	1:B:2092:LEU:HB2	1.95	0.49
2:J:2200:MET:HE3	2:J:2235:TYR:HD1	1.77	0.49
1:B:687:GLN:OE1	1:B:689:TYR:OH	2.19	0.48
1:B:2031:SER:OG	1:B:2097:PRO:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:LEU:HD22	1:B:819:VAL:HB	1.95	0.48
1:B:967:ASN:OD1	1:B:999:GLN:HG3	2.13	0.48
2:J:2197:ALA:HA	2:J:2200:MET:CE	2.43	0.48
1:B:1013:GLU:OE2	1:B:1016:ARG:NH1	2.47	0.48
1:B:1940:LEU:HD22	1:B:2109:MET:HE2	1.95	0.48
1:B:1563:VAL:HG12	1:B:1664:MET:HE2	1.96	0.48
1:B:2065:TRP:CD1	1:B:2081:ARG:HG3	2.49	0.48
1:B:1877:HIS:HE1	1:B:1896:GLN:HB2	1.79	0.48
1:B:1040:LEU:O	1:B:1044:VAL:HG13	2.14	0.47
1:B:1044:VAL:O	2:J:2074:ARG:NH1	2.42	0.47
1:B:2000:THR:O	1:B:2004:ILE:HG23	2.13	0.47
1:B:743:LEU:HD21	1:B:748:LEU:HD22	1.95	0.47
1:B:1909:GLN:O	1:B:1912:THR:OG1	2.27	0.47
1:B:2039:VAL:HG21	1:B:2106:LEU:HD11	1.97	0.47
1:B:1269:ARG:NH1	1:B:1279:GLU:OE1	2.48	0.47
1:B:1295:TYR:OH	1:B:1720:GLU:OE1	2.24	0.47
1:B:1901:ARG:HE	1:B:2055:LEU:HD11	1.80	0.47
1:B:975:LYS:HG3	1:B:976:THR:HG23	1.96	0.47
1:B:1350:ALA:O	1:B:1492:SER:HA	2.15	0.47
1:B:736:ARG:NH1	1:B:773:GLU:HG2	2.29	0.47
1:B:1135:LEU:HD13	1:B:1177:TYR:CD2	2.50	0.47
1:B:2065:TRP:NE1	1:B:2081:ARG:HG3	2.30	0.47
1:B:1456:VAL:HG12	1:B:1490:LEU:O	2.15	0.47
1:B:757:ALA:O	1:B:761:VAL:HG23	2.14	0.47
1:B:1192:PRO:HG3	1:B:1289:LEU:HD11	1.97	0.47
1:B:1661:VAL:O	1:B:1702:CYS:HA	2.14	0.47
2:J:2302:LYS:HD2	2:J:2308:VAL:HG21	1.96	0.46
1:B:832:GLN:NE2	1:B:843:GLU:OE2	2.47	0.46
1:B:1195:ARG:HH11	1:B:1260:GLU:CD	2.24	0.46
1:B:933:PRO:HG3	1:B:943:LEU:HD22	1.97	0.46
1:B:1896:GLN:HA	1:B:1899:LEU:HB2	1.98	0.46
1:B:1146:LYS:HB2	1:B:1148:PHE:CD1	2.50	0.46
1:B:2038:LEU:HD11	1:B:2089:LYS:HE3	1.98	0.46
2:J:2164:PRO:HB3	2:J:2296:LEU:HD11	1.98	0.46
1:B:704:MET:O	1:B:708:VAL:HG12	2.16	0.46
1:B:464:VAL:HG13	1:B:467:LEU:HD12	1.98	0.46
1:B:1456:VAL:CG1	1:B:1491:SER:HB2	2.45	0.45
1:B:1456:VAL:O	1:B:1459:ILE:HG23	2.17	0.45
1:B:2013:ARG:CZ	1:B:2049:GLY:HA3	2.46	0.45
2:J:2243:ASP:HB3	2:J:2248:PRO:HB3	1.98	0.45
1:B:1594:GLU:H	1:B:1594:GLU:CD	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1875:VAL:HG21	1:B:1893:LEU:HD23	1.97	0.45
1:B:1864:GLU:HA	1:B:1864:GLU:OE1	2.17	0.45
2:J:2149:PRO:HB3	2:J:2281:TYR:CE1	2.52	0.45
1:B:705:ASN:HA	1:B:708:VAL:HG12	1.99	0.45
1:B:772:LEU:O	1:B:775:LYS:HB3	2.16	0.45
1:B:730:GLU:OE2	1:B:733:LYS:HD2	2.17	0.45
1:B:1051:SER:OG	1:B:1053:GLU:HG2	2.17	0.45
1:B:1567:LYS:O	1:B:1571:LEU:HG	2.17	0.45
1:B:462:LEU:HD11	1:B:466:LYS:HD3	1.98	0.45
1:B:465:GLU:OE1	1:B:465:GLU:N	2.49	0.45
1:B:999:GLN:NE2	5:B:5933:HOH:O	2.50	0.45
1:B:1900:SER:HB3	1:B:1954:TRP:CZ2	2.51	0.45
1:B:1931:SER:OG	1:B:2079:ILE:HG21	2.17	0.45
1:B:1739:GLU:HG3	1:B:1754:TYR:CE2	2.52	0.44
1:B:607:GLN:O	1:B:607:GLN:HG3	2.17	0.44
1:B:1498:LYS:HE2	1:B:1498:LYS:HB2	1.74	0.44
1:B:1577:LEU:HD23	1:B:1577:LEU:HA	1.81	0.44
1:B:1607:SER:HA	1:B:1610:LYS:HE2	1.99	0.44
1:B:708:VAL:O	1:B:712:ILE:HG12	2.17	0.44
1:B:1515:HIS:O	1:B:1518:VAL:HG22	2.17	0.44
1:B:573:HIS:CE1	1:B:577:LYS:HD3	2.53	0.44
1:B:1383:GLU:O	1:B:1387:GLU:HG2	2.18	0.44
1:B:694:GLU:HG2	1:B:699:LYS:HB3	1.99	0.44
1:B:752:LEU:HG	1:B:759:THR:HG23	2.00	0.44
1:B:1049:LYS:HE2	2:J:2078:ILE:HD13	1.99	0.44
1:B:1170:MET:HA	1:B:1170:MET:HE2	1.98	0.44
1:B:1045:PRO:HD3	2:J:2317:PHE:CD2	2.52	0.44
1:B:1481:ILE:HD12	1:B:1483:ARG:H	1.82	0.44
1:B:1855:TYR:O	1:B:1856:GLU:HG2	2.18	0.44
1:B:1141:LYS:O	1:B:1145:LYS:HG3	2.17	0.43
1:B:1195:ARG:NH1	1:B:1260:GLU:OE1	2.51	0.43
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.99	0.43
1:B:1953:MET:C	1:B:1954:TRP:CD1	2.95	0.43
1:B:1627:MET:HE3	1:B:1627:MET:HB3	1.84	0.43
1:B:1678:ASP:OD1	1:B:1710:LYS:HE3	2.18	0.43
1:B:2076:LEU:HD21	1:B:2079:ILE:HB	2.00	0.43
1:B:639:ILE:O	1:B:643:GLN:N	2.52	0.43
1:B:569:LEU:HD23	1:B:569:LEU:HA	1.80	0.43
1:B:1195:ARG:HD3	1:B:1260:GLU:OE2	2.18	0.43
1:B:1524:GLU:HB2	1:B:1701:ARG:HG2	1.99	0.43
1:B:774:LEU:HD23	1:B:774:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:HIS:HB2	5:B:6220:HOH:O	2.17	0.43
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	2.00	0.43
1:B:1843:ARG:HA	1:B:1846:ILE:HD13	1.99	0.43
1:B:1981:SER:O	1:B:1984:ASP:HB2	2.19	0.43
1:B:436:ARG:HD3	1:B:443:GLU:CD	2.44	0.43
1:B:639:ILE:HD11	1:B:646:VAL:HB	1.99	0.43
1:B:1515:HIS:NE2	1:B:1721:PRO:HG3	2.34	0.43
2:J:2228:TYR:OH	2:J:2258:ARG:NH2	2.44	0.43
1:B:431:PRO:HA	4:B:5803:EDO:H22	2.00	0.43
1:B:763:ARG:HA	1:B:766:ALA:HB3	2.01	0.43
1:B:1601:LEU:O	1:B:1610:LYS:HD3	2.18	0.43
1:B:550:GLU:OE1	1:B:551:MET:HE2	2.19	0.42
1:B:575:LEU:HD21	5:B:6107:HOH:O	2.19	0.42
1:B:1228:VAL:CG2	1:B:1263:PRO:HB2	2.49	0.42
1:B:575:LEU:HD23	1:B:1218:SER:OG	2.20	0.42
1:B:1595:LYS:HB3	1:B:1595:LYS:HE2	1.95	0.42
1:B:1158:HIS:CD2	1:B:1172:LYS:HA	2.47	0.42
1:B:2081:ARG:H	1:B:2081:ARG:HD2	1.83	0.42
1:B:1600:TYR:HD2	1:B:1631:LEU:HD12	1.85	0.42
1:B:469:LYS:HA	1:B:472:GLN:HG3	2.01	0.42
1:B:1937:SER:HB2	1:B:1938:PRO:HD3	2.01	0.42
1:B:2068:ILE:CG2	1:B:2078:SER:HB2	2.50	0.42
1:B:1901:ARG:NE	1:B:2055:LEU:HD11	2.35	0.42
1:B:468:PRO:HB2	1:B:470:TYR:CE1	2.55	0.42
1:B:712:ILE:CD1	1:B:721:VAL:HG21	2.49	0.42
1:B:736:ARG:HG2	1:B:777:LEU:HD21	2.01	0.41
1:B:689:TYR:HE2	1:B:883:LEU:HD12	1.85	0.41
1:B:1967:THR:HG22	1:B:1970:HIS:ND1	2.35	0.41
1:B:438:GLN:C	1:B:439:ARG:HG2	2.45	0.41
1:B:600:GLY:HA3	5:B:6290:HOH:O	2.20	0.41
1:B:1040:LEU:HD13	1:B:1040:LEU:HA	1.79	0.41
1:B:1146:LYS:HB2	1:B:1148:PHE:CE1	2.55	0.41
1:B:1442:ARG:HA	1:B:1442:ARG:HD2	1.59	0.41
1:B:1523:LEU:HD13	1:B:1525:LEU:HB2	2.02	0.41
1:B:1695:LEU:C	1:B:1696:GLN:HG3	2.45	0.41
1:B:1195:ARG:HG3	4:B:5811:EDO:H11	2.03	0.41
1:B:1594:GLU:O	1:B:1598:ILE:HG12	2.20	0.41
1:B:462:LEU:HD11	1:B:466:LYS:HB3	2.01	0.41
1:B:1260:GLU:HA	1:B:1261:PRO:C	2.46	0.41
1:B:1648:ARG:NH2	1:B:1683:ASP:OD2	2.54	0.41
1:B:2077:ILE:HD13	1:B:2094:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2107:PRO:HG2	2:J:2110:VAL:HG22	2.02	0.41
1:B:545:ARG:O	1:B:549:GLN:HG3	2.20	0.41
1:B:637:ARG:HD2	1:B:919:TRP:HA	2.02	0.41
1:B:2081:ARG:HD2	1:B:2081:ARG:N	2.35	0.41
1:B:548:VAL:HG13	1:B:587:VAL:HG12	2.03	0.41
1:B:696:LYS:HB2	1:B:696:LYS:HE2	1.86	0.41
1:B:743:LEU:HD23	1:B:743:LEU:HA	1.86	0.41
1:B:1149:PRO:HD2	1:B:1152:ARG:HD2	2.02	0.41
1:B:1523:LEU:CD1	1:B:1525:LEU:HB2	2.51	0.41
1:B:1539:LEU:HD22	1:B:1664:MET:HE3	2.03	0.41
1:B:2037:VAL:CG1	1:B:2092:LEU:HB2	2.51	0.41
1:B:858:ARG:HA	1:B:859:PRO:HD3	1.89	0.41
1:B:971:LYS:HB2	1:B:980:GLN:HB3	2.03	0.41
1:B:1936:LEU:HB2	1:B:2075:SER:C	2.46	0.41
2:J:2319:LEU:HD12	2:J:2319:LEU:HA	1.94	0.41
1:B:1443:LYS:H	1:B:1443:LYS:CD	2.28	0.40
1:B:1868:LEU:HD23	1:B:1871:LEU:HD12	2.03	0.40
1:B:1926:CYS:O	1:B:1930:LEU:HG	2.21	0.40
1:B:421:HIS:CE1	1:B:843:GLU:HG3	2.56	0.40
1:B:665:LEU:HB2	1:B:667:VAL:HG23	2.01	0.40
1:B:728:ARG:HG2	1:B:786:HIS:CG	2.57	0.40
1:B:2108:PHE:O	1:B:2117:ASP:HA	2.21	0.40
1:B:699:LYS:HE2	1:B:699:LYS:HB2	1.85	0.40
1:B:1922:LEU:HD23	1:B:1922:LEU:HA	1.90	0.40
1:B:1969:GLU:HG3	1:B:1973:ARG:NH1	2.37	0.40
1:B:1871:LEU:HD23	1:B:1874:LYS:NZ	2.36	0.40
1:B:2114:MET:HE3	1:B:2114:MET:HB2	1.86	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	1717/1747 (98%)	1649 (96%)	62 (4%)	6 (0%)	36	30
2	J	261/263 (99%)	248 (95%)	12 (5%)	1 (0%)	30	22
All	All	1978/2010 (98%)	1897 (96%)	74 (4%)	7 (0%)	30	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1859	PRO
2	J	2059	PRO
1	B	1885	ASN
1	B	2028	SER
1	B	2057	PRO
1	B	2097	PRO
1	B	768	GLN

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	1538/1560 (99%)	1474 (96%)	64 (4%)	26	20
2	J	236/236 (100%)	227 (96%)	9 (4%)	29	24
All	All	1774/1796 (99%)	1701 (96%)	73 (4%)	27	21

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	482	ASN
1	B	484	ILE
1	B	487	LYS
1	B	495	THR
1	B	510	THR
1	B	585	ILE
1	B	607	GLN
1	B	696	LYS
1	B	730	GLU

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Mol	Chain	Res	Type
1	B	759	THR
1	B	763	ARG
1	B	789	MET
1	B	790	THR
1	B	791	ARG
1	B	792	VAL
1	B	795	THR
1	B	796	LEU
1	B	812	THR
1	B	863	THR
1	B	877	GLN
1	B	895	SER
1	B	931	ARG
1	B	984	LEU
1	B	987	ILE
1	B	1009	LEU
1	B	1032	GLU
1	B	1040	LEU
1	B	1071	LYS
1	B	1113	ASN
1	B	1126	MET
1	B	1137	GLU
1	B	1139	VAL
1	B	1152	ARG
1	B	1244	LYS
1	B	1313	ARG
1	B	1371	SER
1	B	1400	ARG
1	B	1414	THR
1	B	1416	LEU
1	B	1417	LYS
1	B	1435	LEU
1	B	1443	LYS
1	B	1481	ILE
1	B	1507	SER
1	B	1523	LEU
1	B	1566	ARG
1	B	1586	ARG
1	B	1605	SER
1	B	1614	LEU
1	B	1772	ASN
1	B	1807	GLU

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Mol	Chain	Res	Type
1	B	1831	LEU
1	B	1860	ILE
1	B	1868	LEU
1	B	1885	ASN
1	B	1889	VAL
1	B	1891	THR
1	B	1912	THR
1	B	1953	MET
1	B	1962	GLN
1	B	1996	LEU
1	B	2017	ILE
1	B	2106	LEU
1	B	2116	CYS
2	J	2063	MET
2	J	2072	GLU
2	J	2135	ASP
2	J	2165	GLN
2	J	2225	LEU
2	J	2247	ASN
2	J	2276	GLN
2	J	2289	ASP
2	J	2315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	638	ASN
1	B	643	GLN
1	B	877	GLN
1	B	951	GLN
1	B	1038	GLN
1	B	1101	ASN
1	B	1341	ASN
1	B	1513	ASN
1	B	1692	ASN
1	B	2003	GLN
1	B	2012	ASN
2	J	2158	HIS
2	J	2276	GLN
2	J	2288	HIS
2	J	2291	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	5805	-	3,3,3	0.48	0	2,2,2	0.58	0
4	EDO	B	5810	-	3,3,3	0.62	0	2,2,2	0.33	0
4	EDO	J	2401	-	3,3,3	0.51	0	2,2,2	1.12	0
4	EDO	B	5804	-	3,3,3	0.41	0	2,2,2	1.11	0
4	EDO	B	5807	-	3,3,3	0.54	0	2,2,2	0.41	0
4	EDO	B	5802	-	3,3,3	0.32	0	2,2,2	0.84	0
4	EDO	B	5812	-	3,3,3	0.57	0	2,2,2	0.57	0
3	B09	B	5801	-	11,12,12	1.40	3 (27%)	12,16,16	3.54	3 (25%)
4	EDO	B	5808	-	3,3,3	0.53	0	2,2,2	0.59	0
4	EDO	B	5803	-	3,3,3	0.41	0	2,2,2	0.80	0
4	EDO	B	5809	-	3,3,3	0.54	0	2,2,2	0.86	0
4	EDO	B	5806	-	3,3,3	0.42	0	2,2,2	0.81	0
4	EDO	B	5811	-	3,3,3	0.39	0	2,2,2	0.22	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
4	EDO	B	5805	-	-	0/1/1/1	-
4	EDO	B	5810	-	-	0/1/1/1	-
4	EDO	J	2401	-	-	1/1/1/1	-
4	EDO	B	5804	-	-	1/1/1/1	-
4	EDO	B	5807	-	-	0/1/1/1	-
4	EDO	B	5802	-	-	0/1/1/1	-
4	EDO	B	5812	-	-	1/1/1/1	-
3	B09	B	5801	-	-	0/8/10/10	0/1/1/1
4	EDO	B	5808	-	-	0/1/1/1	-
4	EDO	B	5803	-	-	1/1/1/1	-
4	EDO	B	5809	-	-	1/1/1/1	-
4	EDO	B	5806	-	-	1/1/1/1	-
4	EDO	B	5811	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5801	B09	O1-S1	2.75	1.46	1.43
3	B	5801	B09	C1-S1	2.32	1.80	1.76
3	B	5801	B09	O2-S1	2.31	1.46	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5801	B09	O2-S1-O1	-10.76	106.45	119.52
3	B	5801	B09	O1-S1-C1	4.29	113.40	107.98
3	B	5801	B09	C7-O3-N1	3.18	112.98	109.54

There are no chirality outliers.

All (6) torsion outliers are listed below:

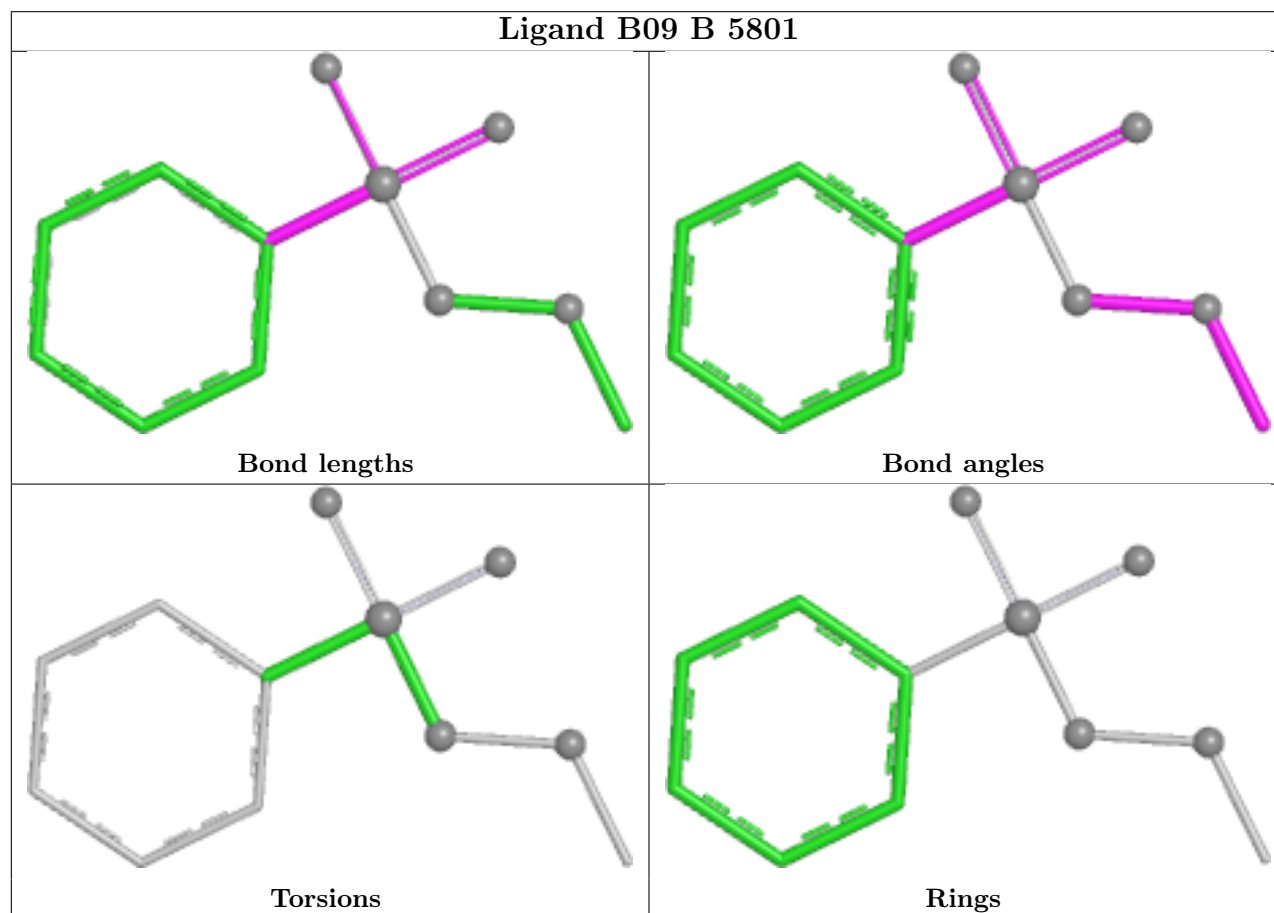
Mol	Chain	Res	Type	Atoms
4	B	5804	EDO	O1-C1-C2-O2
4	B	5812	EDO	O1-C1-C2-O2
4	B	5806	EDO	O1-C1-C2-O2
4	J	2401	EDO	O1-C1-C2-O2
4	B	5809	EDO	O1-C1-C2-O2
4	B	5803	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5802	EDO	1	0
4	B	5803	EDO	1	0
4	B	5809	EDO	1	0
4	B	5811	EDO	4	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, 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	1719/1747 (98%)	0.68	221 (12%) 7 7	26, 55, 128, 176	0
2	J	263/263 (100%)	0.35	17 (6%) 25 24	30, 50, 108, 178	0
All	All	1982/2010 (98%)	0.64	238 (12%) 9 8	26, 54, 128, 178	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1893	LEU	6.3
1	B	404	ALA	5.8
2	J	2320	LEU	5.8
1	B	1875	VAL	5.7
1	B	1860	ILE	5.6
1	B	1894	LEU	5.3
1	B	1165	ILE	5.3
1	B	2095	VAL	5.2
1	B	2036	VAL	5.1
1	B	1877	HIS	5.1
1	B	1954	TRP	4.9
1	B	1868	LEU	4.9
2	J	2319	LEU	4.7
1	B	1936	LEU	4.7
1	B	575	LEU	4.6
1	B	1858	ILE	4.5
2	J	2058	GLY	4.4
1	B	2035	VAL	4.4
2	J	2060	LEU	4.4
1	B	2106	LEU	4.3
1	B	1859	PRO	4.3
1	B	1940	LEU	4.3
1	B	1897	ALA	4.2
1	B	454	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	1871	LEU	4.2
1	B	1906	ALA	4.1
1	B	2039	VAL	4.1
1	B	2077	ILE	4.1
1	B	1879	LEU	4.0
1	B	1887	PRO	4.0
1	B	2038	LEU	4.0
1	B	2068	ILE	3.9
1	B	1836	LEU	3.9
1	B	1935	TRP	3.9
1	B	766	ALA	3.8
1	B	1904	LEU	3.8
1	B	2097	PRO	3.8
1	B	1895	LEU	3.7
1	B	1908	LEU	3.7
1	B	860	GLN	3.7
1	B	2107	TYR	3.7
2	J	2097	ILE	3.7
1	B	482	ASN	3.6
1	B	1849	ILE	3.6
1	B	2041	LEU	3.6
1	B	1863	HIS	3.6
1	B	2102	HIS	3.6
2	J	2317	PHE	3.5
1	B	762	LEU	3.5
1	B	456	GLY	3.5
1	B	1891	THR	3.5
1	B	782	PHE	3.4
1	B	403	LEU	3.4
1	B	2104	TYR	3.4
1	B	1584	ILE	3.4
1	B	1938	PRO	3.4
1	B	2108	PHE	3.4
1	B	455	PHE	3.3
1	B	1959	TYR	3.3
1	B	1838	ALA	3.3
1	B	1872	ALA	3.3
1	B	2105	THR	3.3
1	B	1515	HIS	3.3
1	B	1842	VAL	3.3
1	B	1889	VAL	3.3
1	B	2067	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	2120	TYR	3.3
1	B	1941	ALA	3.3
2	J	2318	ALA	3.3
1	B	1996	LEU	3.3
1	B	2092	LEU	3.3
1	B	1600	TYR	3.2
1	B	2029	ILE	3.2
1	B	1892	ASN	3.2
2	J	2286	VAL	3.2
1	B	2021	TYR	3.2
1	B	761	VAL	3.1
1	B	1979	VAL	3.1
1	B	2023	VAL	3.1
1	B	2037	VAL	3.1
1	B	1598	ILE	3.1
1	B	405	PRO	3.1
1	B	1837	ASN	3.1
1	B	2082	LEU	3.1
1	B	1846	ILE	3.1
1	B	605	TYR	3.1
1	B	1845	LEU	3.1
1	B	571	GLY	3.0
1	B	1886	ASP	3.0
1	B	2028	SER	3.0
1	B	2075	SER	3.0
1	B	1153	LEU	3.0
1	B	1885	ASN	3.0
1	B	1971	ILE	2.9
1	B	1866	ASN	2.9
1	B	2096	ALA	2.9
1	B	1999	LEU	2.9
2	J	2061	GLY	2.9
1	B	726	HIS	2.9
1	B	1896	GLN	2.9
2	J	2063	MET	2.9
2	J	2062	SER	2.9
1	B	1899	LEU	2.9
1	B	1848	ILE	2.9
1	B	1861	ARG	2.9
1	B	2017	ILE	2.9
1	B	1884	PHE	2.9
1	B	1890	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	603	ARG	2.8
1	B	1873	GLN	2.8
1	B	812	THR	2.8
1	B	2099	THR	2.8
1	B	1044	VAL	2.8
1	B	1878	LYS	2.8
1	B	748	LEU	2.8
1	B	759	THR	2.8
1	B	2004	ILE	2.8
1	B	757	ALA	2.7
1	B	2019	LEU	2.7
1	B	2090	VAL	2.7
1	B	1995	ALA	2.7
1	B	764	THR	2.7
1	B	1156	LEU	2.7
2	J	2059	PRO	2.7
1	B	2047	VAL	2.7
1	B	1915	ILE	2.7
1	B	2065	TRP	2.7
1	B	774	LEU	2.7
1	B	2000	THR	2.7
1	B	573	HIS	2.7
1	B	780	TYR	2.7
1	B	1902	MET	2.6
1	B	1945	LEU	2.6
2	J	2120	LEU	2.6
1	B	1985	ILE	2.6
1	B	755	GLY	2.6
2	J	2100	THR	2.6
1	B	2034	PRO	2.6
1	B	1953	MET	2.6
1	B	2101	ALA	2.6
1	B	1876	PRO	2.6
1	B	1867	LEU	2.6
1	B	2040	GLN	2.5
1	B	459	GLU	2.5
1	B	703	ILE	2.5
1	B	777	LEU	2.5
1	B	1929	VAL	2.5
1	B	861	TYR	2.5
1	B	574	GLN	2.5
1	B	787	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	752	LEU	2.5
1	B	701	PHE	2.5
1	B	1140	VAL	2.5
1	B	1164	LEU	2.5
1	B	1834	MET	2.5
1	B	576	CYS	2.4
1	B	863	THR	2.4
1	B	2033	GLY	2.4
2	J	2101	GLY	2.4
1	B	1143	ILE	2.4
1	B	2066	VAL	2.4
1	B	461	LEU	2.4
1	B	1601	LEU	2.4
1	B	1857	ASN	2.4
1	B	751	PHE	2.4
1	B	1932	SER	2.4
1	B	1592	CYS	2.4
1	B	1912	THR	2.4
1	B	1930	LEU	2.4
2	J	2285	GLY	2.4
1	B	2091	LYS	2.4
1	B	743	LEU	2.3
1	B	1070	LEU	2.3
1	B	2076	LEU	2.3
1	B	763	ARG	2.3
1	B	1927	VAL	2.3
1	B	1937	SER	2.3
1	B	769	CYS	2.3
1	B	1167	MET	2.3
1	B	1835	SER	2.3
1	B	725	VAL	2.3
1	B	1964	PRO	2.3
1	B	1483	ARG	2.3
1	B	2069	GLY	2.3
1	B	457	SER	2.3
1	B	779	PRO	2.3
1	B	1731	CYS	2.3
1	B	783	ALA	2.3
1	B	2071	ALA	2.3
1	B	527	MET	2.3
1	B	640	GLU	2.2
1	B	2031	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2024	VAL	2.2
1	B	1880	ASN	2.2
1	B	641	MET	2.2
1	B	1939	ALA	2.2
1	B	1914	GLU	2.2
1	B	727	SER	2.2
1	B	2078	SER	2.2
1	B	604	THR	2.2
1	B	1840	THR	2.2
1	B	2079	ILE	2.2
1	B	2103	ASN	2.2
1	B	1949	VAL	2.2
1	B	1599	PRO	2.2
1	B	1966	PHE	2.2
1	B	792	VAL	2.2
1	B	1850	SER	2.2
1	B	1933	ASN	2.2
1	B	600	GLY	2.1
1	B	805	HIS	2.1
1	B	778	LEU	2.1
1	B	1910	SER	2.1
1	B	2001	ASP	2.1
1	B	525	ILE	2.1
1	B	1481	ILE	2.1
1	B	2094	PHE	2.1
1	B	1965	HIS	2.1
1	B	1833	SER	2.1
1	B	1900	SER	2.1
2	J	2095	ASP	2.1
1	B	698	ILE	2.1
1	B	1442	ARG	2.1
1	B	2112	ALA	2.1
1	B	796	LEU	2.1
1	B	1955	SER	2.1
1	B	1856	GLU	2.1
1	B	1139	VAL	2.1
1	B	735	ALA	2.1
1	B	750	LEU	2.0
1	B	1963	LEU	2.0
1	B	1843	ARG	2.0
1	B	806	ILE	2.0
1	B	1869	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	1901	ARG	2.0
1	B	1956	LYS	2.0
1	B	790	THR	2.0
1	B	1719	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

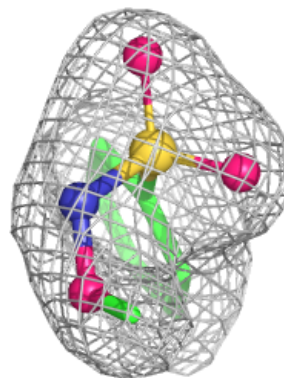
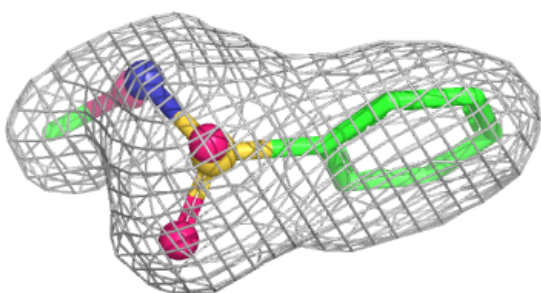
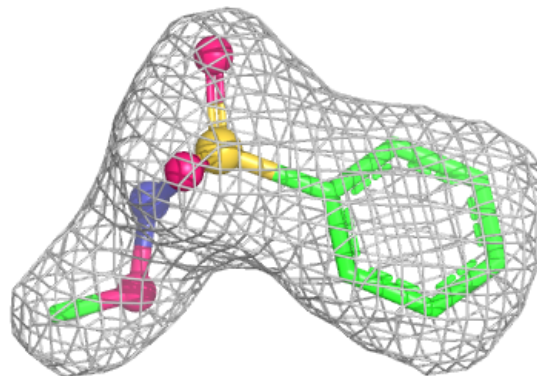
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	5810	4/4	0.67	0.15	53,56,57,63	0
4	EDO	B	5807	4/4	0.72	0.14	59,59,60,68	0
4	EDO	B	5808	4/4	0.74	0.17	49,50,54,55	0
4	EDO	B	5805	4/4	0.80	0.17	64,64,64,65	0
4	EDO	B	5802	4/4	0.80	0.15	38,40,48,49	0
4	EDO	B	5806	4/4	0.84	0.14	56,59,60,64	0
4	EDO	B	5809	4/4	0.85	0.13	32,40,41,44	0
4	EDO	B	5811	4/4	0.86	0.13	47,52,52,55	0
4	EDO	J	2401	4/4	0.86	0.12	42,46,49,51	0
4	EDO	B	5803	4/4	0.88	0.14	54,55,61,67	0
4	EDO	B	5804	4/4	0.91	0.14	48,48,49,50	0
4	EDO	B	5812	4/4	0.92	0.10	42,50,54,57	0
3	B09	B	5801	12/12	0.97	0.08	37,44,46,46	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 B09 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.