



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:43 AM UTC

PDB ID : 8BC9 / pdb_00008bc9
Title : Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and compound 24
Authors : Vester, K.; Loll, B.; Wahl, M.C.
Deposited on : 2022-10-15
Resolution : 2.30 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

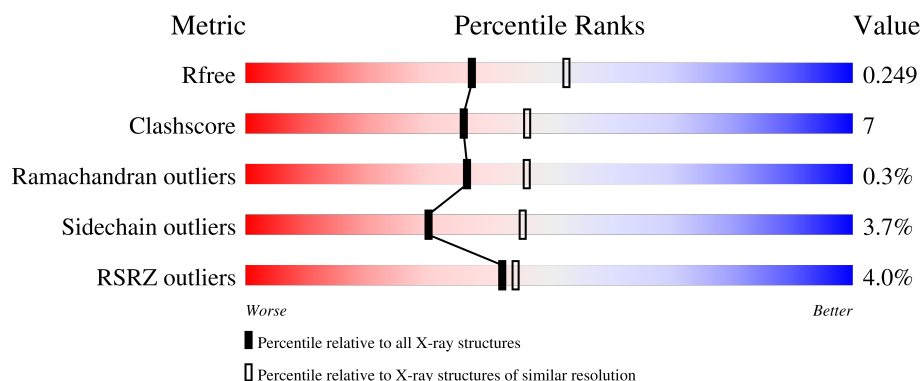
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	4% 78% 19% ..
2	J	263	5% 81% 17% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16458 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	1724	Total	C	N	O	S	0	0	0
			13862	8859	2372	2559	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

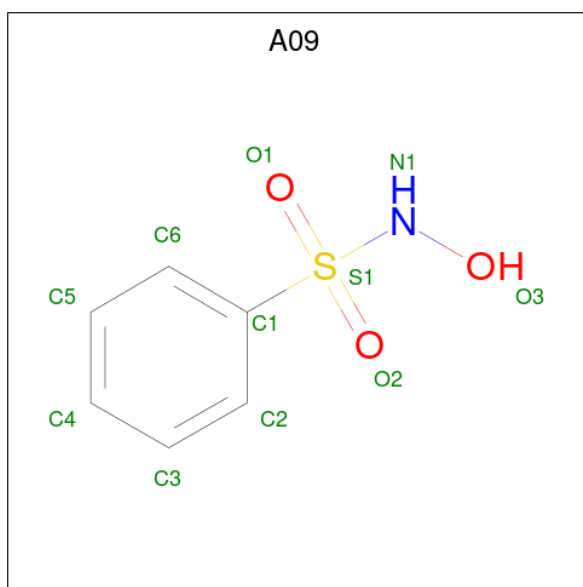
- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

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:

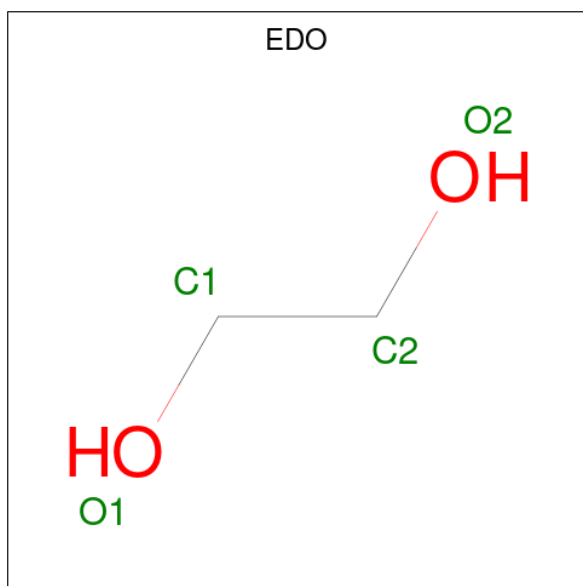
Chain	Residue	Modelled	Actual	Comment	Reference
J	2058	GLY	-	expression tag	UNP Q6P2Q9
J	2059	PRO	-	expression tag	UNP Q6P2Q9
J	2060	LEU	-	expression tag	UNP Q6P2Q9
J	2061	GLY	-	expression tag	UNP Q6P2Q9
J	2062	SER	-	expression tag	UNP Q6P2Q9
J	2063	MET	-	expression tag	UNP Q6P2Q9

- Molecule 3 is N-hydroxybenzenesulfonamide (CCD ID: A09) (formula: C₆H₇NO₃S) (labeled as "Ligand of Interest" by depositor).



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

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



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	J	1	Total C O 4 2 2	0	0

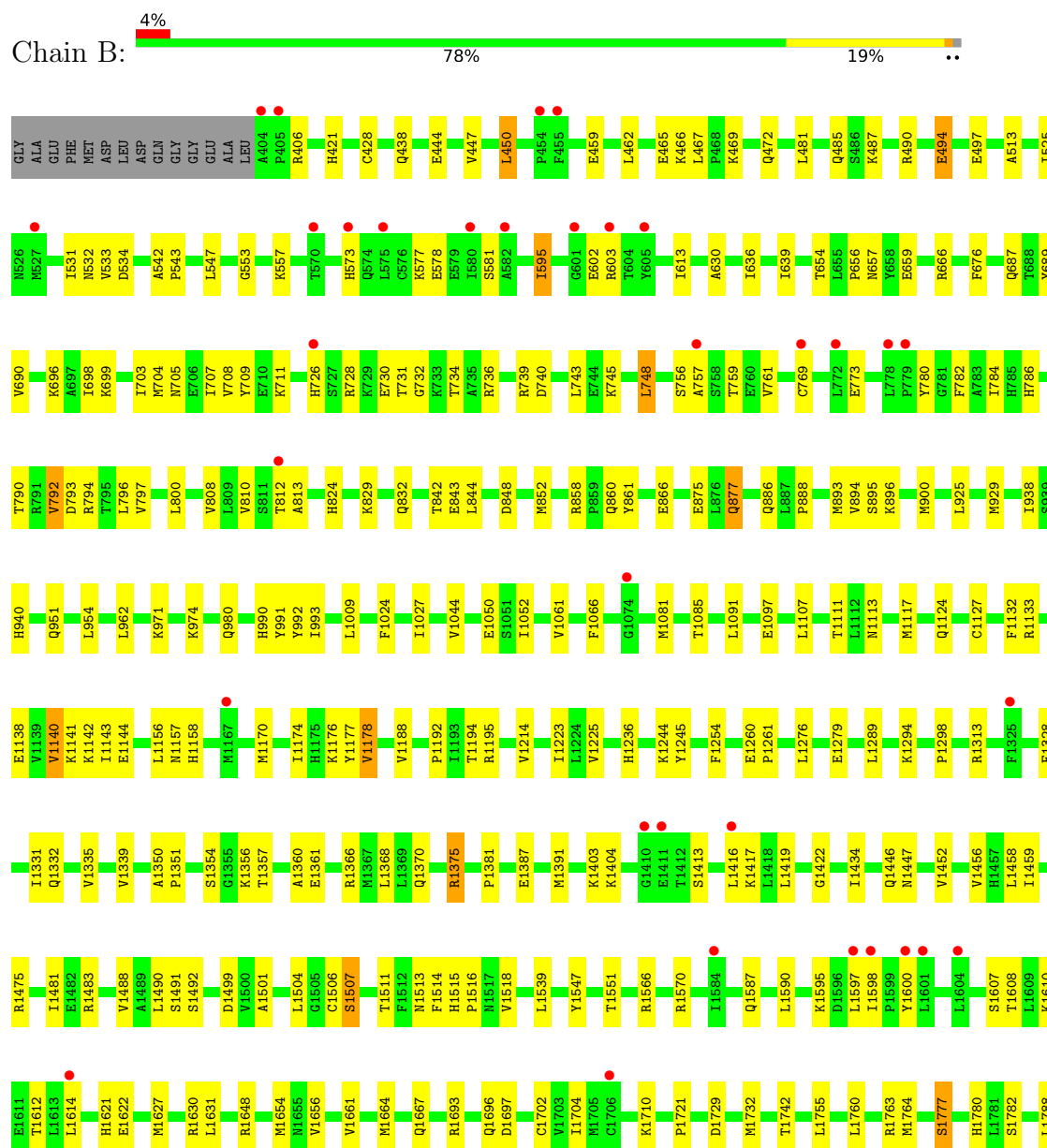
- Molecule 5 is water.

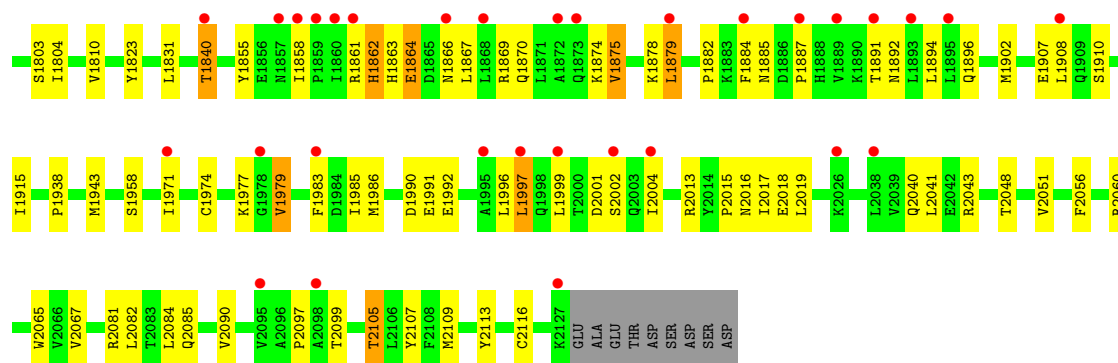
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	360	Total O 360 360	0	13
5	J	58	Total O 58 58	0	1

3 Residue-property plots

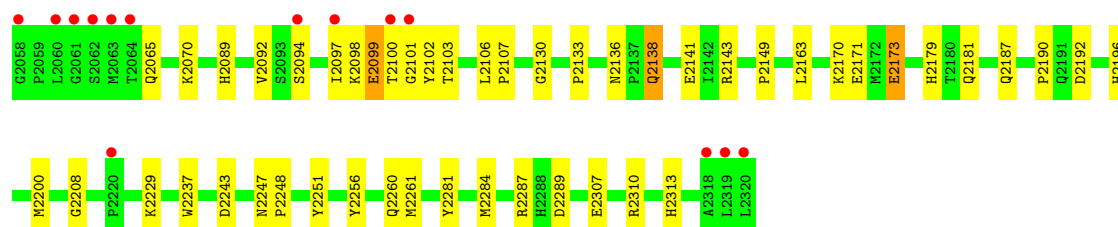
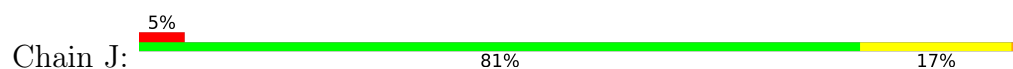
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: U5 small nuclear ribonucleoprotein 200 kDa helicase





• 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	99.83Å 119.22Å 188.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.04 – 2.30 46.04 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.04-2.30) 99.9 (46.04-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.198 , 0.249 0.198 , 0.249	Depositor DCC
R_{free} test set	2101 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16458	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: A09, 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	0.35	0/14156	0.53	0/19180
2	J	0.36	0/2190	0.53	0/2981
All	All	0.35	0/16346	0.53	0/22161

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	13862	0	14007	205	1
2	J	2123	0	2063	29	1
3	B	11	0	7	0	0
4	B	40	0	60	5	0
4	J	4	0	6	0	0
5	B	360	0	0	10	0
5	J	58	0	0	1	0
All	All	16458	0	16143	235	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 7.

All (235) 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:406:ARG:NH2	1:B:951:GLN:OE1	2.07	0.88
1:B:1595:LYS:HA	1:B:1598:ILE:HD12	1.65	0.76
2:J:2200:MET:HE2	2:J:2208:GLY:HA2	1.69	0.75
1:B:1404:LYS:HB3	1:B:1422:GLY:HA2	1.70	0.73
1:B:1977:LYS:HD3	1:B:1996:LEU:HD13	1.70	0.72
1:B:1475:ARG:HD2	1:B:1504:LEU:HA	1.71	0.72
1:B:462:LEU:HD11	1:B:466:LYS:HG2	1.70	0.72
2:J:2100:THR:HG21	2:J:2229:LYS:HD3	1.72	0.71
1:B:1696:GLN:OE1	5:B:5901:HOH:O	2.10	0.68
1:B:1600:TYR:HB3	1:B:1631:LEU:HD11	1.77	0.66
2:J:2196:HIS:CD2	2:J:2200:MET:HE3	2.30	0.65
1:B:573:HIS:HB3	1:B:577:LYS:HG3	1.78	0.65
1:B:1760:LEU:HD11	1:B:1764:MET:HE3	1.78	0.65
2:J:2200:MET:CE	2:J:2208:GLY:HA2	2.28	0.64
2:J:2196:HIS:NE2	2:J:2200:MET:HE3	2.12	0.63
1:B:2001:ASP:O	1:B:2004:ILE:HG13	1.98	0.63
1:B:467:LEU:HD21	1:B:481:LEU:HD11	1.80	0.63
1:B:1066:PHE:HD1	1:B:1081:MET:HE3	1.64	0.62
1:B:1024:PHE:HB3	1:B:1027:ILE:HD12	1.82	0.62
1:B:993:ILE:HD12	1:B:1091:LEU:HD23	1.81	0.61
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.82	0.61
1:B:1456:VAL:HG12	1:B:1491:SER:HB2	1.83	0.61
2:J:2133:PRO:HG2	2:J:2136:ASN:HB2	1.83	0.61
1:B:2015:PRO:HG2	1:B:2116:CYS:SG	2.42	0.60
1:B:1174:ILE:O	1:B:1178:VAL:HG13	2.02	0.60
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	1.82	0.60
1:B:1194:THR:HB	4:B:5806:EDO:H11	1.83	0.60
2:J:2196:HIS:HE2	2:J:2200:MET:HE3	1.66	0.60
1:B:991:TYR:OH	1:B:1097:GLU:OE1	2.17	0.59
1:B:1107:LEU:O	1:B:1111:THR:HG23	2.01	0.59
1:B:893:MET:HG2	1:B:925:LEU:HB2	1.85	0.59
1:B:860:GLN:N	1:B:860:GLN:OE1	2.36	0.58
1:B:2082:LEU:HD22	1:B:2090:VAL:HG21	1.84	0.58
1:B:1507:SER:O	1:B:1511:THR:HG23	2.02	0.58
1:B:630:ALA:HB2	1:B:900:MET:HE3	1.85	0.58
1:B:1943:MET:HE3	1:B:2065:TRP:HB2	1.85	0.58
1:B:1693:ARG:HD3	1:B:1697:ASP:OD2	2.02	0.57
2:J:2187:GLN:HB2	2:J:2256:TYR:OH	2.02	0.57
1:B:1879:LEU:HD23	1:B:1879:LEU:H	1.69	0.56
1:B:1050:GLU:CD	1:B:1050:GLU:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1298:PRO:HB3	1:B:1515:HIS:CG	2.40	0.56
1:B:1335:VAL:O	1:B:1339:VAL:HG23	2.05	0.56
1:B:1551:THR:HG22	1:B:1587:GLN:OE1	2.05	0.55
1:B:1866:ASN:HA	1:B:1869:ARG:HB2	1.88	0.55
1:B:1192:PRO:HG3	1:B:1289:LEU:HD11	1.87	0.55
1:B:731:THR:HG21	1:B:786:HIS:HD2	1.72	0.55
1:B:1974:CYS:HA	1:B:1996:LEU:HD21	1.88	0.55
1:B:421:HIS:NE2	1:B:875:GLU:OE1	2.28	0.55
1:B:1413:SER:HA	1:B:1416:LEU:HD12	1.89	0.55
1:B:1943:MET:HG2	1:B:2065:TRP:CE3	2.42	0.54
2:J:2141:GLU:OE1	2:J:2143:ARG:NH2	2.40	0.54
1:B:894:VAL:HG22	5:B:6041:HOH:O	2.08	0.54
1:B:1943:MET:HE2	1:B:2109:MET:HB2	1.89	0.54
1:B:2013:ARG:HE	1:B:2048:THR:HG23	1.73	0.54
1:B:532:ASN:C	1:B:534:ASP:H	2.17	0.53
1:B:1874:LYS:O	1:B:1902:MET:HE1	2.07	0.53
1:B:1368:LEU:HD22	1:B:1403:LYS:HE2	1.89	0.53
1:B:602:GLU:HG3	1:B:603:ARG:H	1.74	0.53
1:B:1875:VAL:HG22	1:B:1896:GLN:HB3	1.91	0.53
1:B:1298:PRO:HB3	1:B:1515:HIS:CD2	2.44	0.53
1:B:1654:MET:HG2	1:B:1656:VAL:HG22	1.92	0.52
1:B:1127:CYS:HB2	1:B:1144:GLU:HG3	1.89	0.52
1:B:1157:ASN:OD1	1:B:1158:HIS:N	2.36	0.52
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	1.91	0.52
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.45	0.51
1:B:2067:VAL:HB	1:B:2107:TYR:HB2	1.91	0.51
1:B:1515:HIS:HB3	1:B:1516:PRO:HD2	1.92	0.51
1:B:490:ARG:HA	1:B:494:GLU:HG3	1.92	0.51
1:B:1195:ARG:HD3	1:B:1260:GLU:OE2	2.10	0.51
1:B:1539:LEU:HD22	1:B:1664:MET:HE3	1.92	0.51
1:B:962:LEU:HD21	1:B:974:LYS:HE2	1.93	0.51
1:B:687:GLN:OE1	1:B:689:TYR:OH	2.12	0.51
1:B:734:THR:HG21	1:B:829:LYS:HE2	1.93	0.51
1:B:1879:LEU:HG	1:B:1882:PRO:HB3	1.93	0.51
1:B:1974:CYS:HB3	1:B:1979:VAL:HB	1.93	0.51
1:B:726:HIS:CE1	1:B:844:LEU:HD11	2.46	0.51
1:B:1566:ARG:HG3	1:B:1621:HIS:CG	2.46	0.50
1:B:542:ALA:HB1	1:B:547:LEU:HD23	1.93	0.50
1:B:929:MET:HE3	1:B:938:ILE:HD11	1.94	0.50
1:B:1481:ILE:HG13	1:B:1483:ARG:H	1.75	0.50
1:B:602:GLU:HB3	5:B:6211:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:971:LYS:HB2	1:B:980:GLN:HB3	1.93	0.50
1:B:1357:THR:O	1:B:1361:GLU:HG3	2.12	0.50
1:B:728:ARG:O	1:B:731:THR:HG22	2.11	0.50
2:J:2092:VAL:HG13	2:J:2261:MET:HE3	1.93	0.50
1:B:980:GLN:NE2	5:B:5912:HOH:O	2.43	0.49
1:B:1570:ARG:NH2	1:B:1608:THR:OG1	2.45	0.49
1:B:1879:LEU:H	1:B:1879:LEU:CD2	2.25	0.49
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.93	0.49
1:B:748:LEU:HD21	1:B:780:TYR:HB3	1.94	0.49
1:B:1132:PHE:HE1	1:B:1214:VAL:HG11	1.77	0.49
1:B:699:LYS:O	1:B:703:ILE:HG13	2.12	0.49
1:B:900:MET:HG2	5:B:6207:HOH:O	2.13	0.49
1:B:1894:LEU:HD21	1:B:1908:LEU:HD22	1.93	0.49
1:B:1113:ASN:O	1:B:1117:MET:HG3	2.12	0.48
1:B:1983:PHE:CD1	1:B:1986:MET:HE1	2.48	0.48
1:B:812:THR:OG1	1:B:813:ALA:N	2.46	0.48
1:B:654:THR:HG21	1:B:676:PHE:O	2.13	0.48
1:B:1434:ILE:HD12	1:B:1823:TYR:HB2	1.94	0.48
2:J:2103:THR:HG23	2:J:2260:GLN:HG2	1.94	0.48
1:B:1777:SER:HB3	1:B:1780:HIS:ND1	2.29	0.48
1:B:1861:ARG:HH12	1:B:1907:GLU:HB3	1.78	0.48
1:B:739:ARG:NE	1:B:740:ASP:OD1	2.38	0.48
4:B:5806:EDO:H22	5:B:6078[B]:HOH:O	2.12	0.48
1:B:462:LEU:HD11	1:B:466:LYS:CG	2.42	0.48
1:B:578:GLU:O	1:B:581:SER:OG	2.25	0.47
1:B:1729:ASP:OD1	1:B:1729:ASP:N	2.47	0.47
1:B:1977:LYS:NZ	1:B:1992:GLU:HG2	2.29	0.47
4:B:5802:EDO:H12	5:B:6199:HOH:O	2.14	0.47
2:J:2179:HIS:CE1	2:J:2181:GLN:HG3	2.49	0.47
1:B:1366:ARG:O	1:B:1370:GLN:HG2	2.15	0.47
1:B:1943:MET:HE3	1:B:2065:TRP:CB	2.44	0.47
2:J:2100:THR:O	2:J:2102:TYR:N	2.41	0.47
1:B:1661:VAL:O	1:B:1702:CYS:HA	2.14	0.47
2:J:2089:HIS:NE2	5:J:2501:HOH:O	2.36	0.47
1:B:1864:GLU:O	1:B:1867:LEU:HB3	2.14	0.47
1:B:1840:THR:O	1:B:1938:PRO:HB3	2.15	0.47
1:B:1977:LYS:HZ2	1:B:1992:GLU:HG2	1.79	0.47
1:B:790:THR:HG22	1:B:792:VAL:H	1.79	0.47
1:B:1506:CYS:HB3	1:B:1511:THR:HG22	1.97	0.47
1:B:1943:MET:HG2	1:B:2065:TRP:CZ3	2.50	0.47
1:B:1943:MET:HE2	1:B:2109:MET:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2243:ASP:HB3	2:J:2248:PRO:HB3	1.98	0.46
1:B:513:ALA:HB1	1:B:613:ILE:HD13	1.97	0.46
1:B:1501:ALA:HB1	1:B:1506:CYS:HB2	1.98	0.46
1:B:1225:VAL:HG21	1:B:1254:PHE:CE2	2.50	0.46
1:B:1882:PRO:HB2	1:B:1884:PHE:CZ	2.51	0.46
1:B:1990:ASP:OD1	1:B:1991:GLU:N	2.48	0.46
1:B:790:THR:HG22	1:B:792:VAL:N	2.30	0.46
1:B:893:MET:HE3	1:B:900:MET:SD	2.55	0.46
1:B:1356:LYS:HB2	4:B:5802:EDO:H21	1.98	0.46
1:B:1732:MET:HE2	1:B:1732:MET:HB2	1.62	0.46
1:B:1887:PRO:O	1:B:1891:THR:HG23	2.15	0.46
1:B:406:ARG:NE	1:B:954:LEU:HG	2.31	0.46
1:B:707:ILE:O	1:B:711:LYS:HG2	2.15	0.46
1:B:497:GLU:HG3	5:B:5918:HOH:O	2.15	0.45
1:B:1375:ARG:HD3	1:B:1419:LEU:O	2.16	0.45
1:B:1710:LYS:HG2	5:B:5990:HOH:O	2.15	0.45
2:J:2284:MET:HE3	2:J:2284:MET:HB2	1.75	0.45
1:B:636:ILE:O	1:B:639:ILE:HB	2.16	0.45
1:B:1294:LYS:HG3	4:B:5806:EDO:O2	2.16	0.45
1:B:1958:SER:HB3	1:B:1971:ILE:HD13	1.99	0.45
2:J:2106:LEU:HD12	2:J:2107:PRO:HD2	1.98	0.45
1:B:1381:PRO:HG2	1:B:1458:LEU:HD12	1.97	0.45
1:B:2056:PHE:CE2	1:B:2060:ARG:HD3	2.51	0.45
1:B:756:SER:HB2	1:B:759:THR:HG23	1.98	0.45
1:B:1138:GLU:O	1:B:1142:LYS:HG3	2.16	0.45
1:B:2017:ILE:HD12	1:B:2084:LEU:HD23	1.98	0.45
1:B:543:PRO:HD2	1:B:547:LEU:HD23	1.98	0.45
1:B:1124:GLN:HB2	2:J:2307:GLU:OE1	2.16	0.45
1:B:1350:ALA:O	1:B:1492:SER:HA	2.16	0.45
1:B:1590:LEU:HD22	1:B:1614:LEU:O	2.17	0.45
1:B:1804:ILE:HG12	1:B:1810:VAL:HG12	1.98	0.45
1:B:636:ILE:HD13	1:B:666:ARG:HG2	1.98	0.44
1:B:1627:MET:HE3	1:B:1627:MET:HB3	1.85	0.44
1:B:447:VAL:HB	1:B:687:GLN:HB2	1.98	0.44
1:B:709:TYR:OH	1:B:745:LYS:HE2	2.18	0.44
2:J:2070:LYS:HB3	2:J:2070:LYS:HE3	1.64	0.44
1:B:469:LYS:HA	1:B:472:GLN:HG3	1.99	0.44
1:B:1170:MET:HA	1:B:1170:MET:HE2	1.99	0.44
1:B:2051:VAL:HG13	1:B:2113:TYR:CZ	2.52	0.44
1:B:704:MET:O	1:B:708:VAL:HG12	2.17	0.44
1:B:1693:ARG:HB3	1:B:1696:GLN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2065:TRP:CD1	1:B:2081:ARG:HG2	2.53	0.44
1:B:1622:GLU:OE1	1:B:1622:GLU:N	2.43	0.44
2:J:2149:PRO:HB3	2:J:2281:TYR:CE1	2.53	0.44
1:B:824:HIS:HE1	1:B:866:GLU:OE2	2.00	0.43
1:B:1452:VAL:HG22	1:B:1488:VAL:HB	1.99	0.43
1:B:481:LEU:HB3	1:B:485:GLN:HB2	2.00	0.43
1:B:690:VAL:HG11	1:B:707:ILE:HD13	1.99	0.43
1:B:769:CYS:SG	1:B:796:LEU:HD22	2.58	0.43
1:B:2017:ILE:HD13	1:B:2043:ARG:HG3	2.01	0.43
2:J:2100:THR:CG2	2:J:2229:LYS:HD3	2.44	0.43
1:B:450:LEU:HA	1:B:450:LEU:HD13	1.77	0.43
1:B:1260:GLU:HA	1:B:1261:PRO:C	2.43	0.43
1:B:1375:ARG:NH1	1:B:1447:ASN:OD1	2.51	0.43
1:B:1515:HIS:CE1	1:B:1721:PRO:HG3	2.53	0.43
1:B:444:GLU:HG2	1:B:690:VAL:HG22	1.99	0.43
1:B:790:THR:O	1:B:794:ARG:HG3	2.19	0.43
1:B:848:ASP:HB3	1:B:852:MET:HE3	2.01	0.43
1:B:2043:ARG:NH2	1:B:2084:LEU:O	2.35	0.43
1:B:553:GLY:O	1:B:557:LYS:HG3	2.18	0.43
1:B:1176:LYS:HG3	1:B:1177:TYR:N	2.33	0.43
1:B:1862:HIS:HE2	1:B:1885:ASN:HB3	1.83	0.43
2:J:2190:PRO:HB3	2:J:2251:TYR:CD1	2.54	0.43
1:B:1223:ILE:O	1:B:1236:HIS:HA	2.18	0.42
1:B:1608:THR:O	1:B:1612:THR:HG23	2.19	0.42
1:B:743:LEU:HB3	1:B:748:LEU:HD12	2.00	0.42
1:B:1597:LEU:HD23	1:B:1614:LEU:HA	2.00	0.42
1:B:1630:ARG:HD2	1:B:1630:ARG:N	2.33	0.42
1:B:736:ARG:NH1	1:B:773:GLU:OE2	2.42	0.42
1:B:784:ILE:HA	1:B:810:VAL:O	2.19	0.42
1:B:796:LEU:HG	1:B:800:LEU:HD13	2.01	0.42
2:J:2163:LEU:HA	2:J:2163:LEU:HD23	1.66	0.42
1:B:428:CYS:HB3	1:B:877:GLN:OE1	2.20	0.42
1:B:1244:LYS:HE3	1:B:1245:TYR:CE2	2.55	0.42
1:B:1943:MET:HE3	1:B:2065:TRP:CG	2.55	0.42
2:J:2136:ASN:HB3	2:J:2138:GLN:OE1	2.19	0.42
1:B:1140:VAL:HA	1:B:1143:ILE:HD12	2.01	0.42
1:B:1755:LEU:HD23	1:B:1755:LEU:HA	1.90	0.42
1:B:1547:TYR:O	1:B:1551:THR:HG23	2.20	0.42
1:B:459:GLU:OE2	1:B:487:LYS:HE2	2.20	0.42
1:B:705:ASN:OD1	1:B:829:LYS:NZ	2.52	0.42
2:J:2179:HIS:NE2	2:J:2192:ASP:OD2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1456:VAL:O	1:B:1459:ILE:HG12	2.20	0.41
1:B:730:GLU:O	1:B:734:THR:HG23	2.20	0.41
1:B:1044:VAL:HG11	1:B:1061:VAL:HG22	2.00	0.41
1:B:656:PRO:O	1:B:657:ASN:HB2	2.21	0.41
1:B:886:GLN:O	1:B:888:PRO:HD3	2.20	0.41
1:B:1983:PHE:HE1	1:B:2016:ASN:HD22	1.67	0.41
1:B:2019:LEU:HD12	1:B:2041:LEU:HD11	2.01	0.41
1:B:1417:LYS:HA	1:B:1417:LYS:HD3	1.58	0.41
1:B:731:THR:HG23	1:B:732:GLY:N	2.35	0.41
1:B:1997:LEU:HD21	1:B:1999:LEU:HB2	2.02	0.41
1:B:782:PHE:HA	1:B:808:VAL:O	2.20	0.41
2:J:2310:ARG:HD2	2:J:2313:HIS:ND1	2.35	0.41
1:B:1499:ASP:OD2	1:B:1763:ARG:NH1	2.51	0.41
1:B:793:ASP:O	1:B:797:VAL:HG23	2.21	0.41
1:B:1328:PHE:HB3	1:B:1332:GLN:HB2	2.03	0.41
1:B:1870:GLN:O	1:B:1874:LYS:HG2	2.20	0.41
1:B:757:ALA:O	1:B:761:VAL:HG23	2.21	0.41
1:B:832:GLN:NE2	1:B:843:GLU:OE2	2.46	0.41
1:B:1878:LYS:HA	1:B:1878:LYS:HD3	1.76	0.41
2:J:2097:ILE:C	2:J:2099:GLU:H	2.29	0.41
1:B:858:ARG:HE	1:B:861:TYR:HB2	1.86	0.40
1:B:1387:GLU:O	1:B:1391:MET:HG2	2.21	0.40
1:B:595:ILE:HD11	1:B:990:HIS:O	2.21	0.40
1:B:896:LYS:HE3	5:B:6114:HOH:O	2.21	0.40
1:B:2105:THR:OG1	1:B:2107:TYR:CZ	2.71	0.40
1:B:1132:PHE:CE1	1:B:1214:VAL:HG11	2.56	0.40
1:B:1855:TYR:CE1	1:B:1915:ILE:HA	2.56	0.40
1:B:1607:SER:O	1:B:1610:LYS:HB2	2.22	0.40
1:B:1803:SER:O	1:B:1810:VAL:HA	2.21	0.40
2:J:2130:GLY:O	2:J:2173:GLU:HG3	2.21	0.40
2:J:2237:TRP:CZ2	2:J:2251:TYR:HB2	2.56	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:1782:SER:OG	2:J:2065:GLN:OE1[4_555]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1722/1747 (99%)	1668 (97%)	50 (3%)	4 (0%)	43	55
2	J	261/263 (99%)	249 (95%)	11 (4%)	1 (0%)	30	38
All	All	1983/2010 (99%)	1917 (97%)	61 (3%)	5 (0%)	36	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2099	THR
2	J	2101	GLY
1	B	2085	GLN
1	B	533	VAL
1	B	2097	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	1543/1560 (99%)	1488 (96%)	55 (4%)	31	47
2	J	236/236 (100%)	226 (96%)	10 (4%)	26	40
All	All	1779/1796 (99%)	1714 (96%)	65 (4%)	30	45

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	438	GLN

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Mol	Chain	Res	Type
1	B	450	LEU
1	B	465	GLU
1	B	494	GLU
1	B	525	ILE
1	B	531	ILE
1	B	595	ILE
1	B	659	GLU
1	B	696	LYS
1	B	698	ILE
1	B	748	LEU
1	B	792	VAL
1	B	842	THR
1	B	877	GLN
1	B	895	SER
1	B	940	HIS
1	B	992	TYR
1	B	1009	LEU
1	B	1052	ILE
1	B	1133	ARG
1	B	1140	VAL
1	B	1141	LYS
1	B	1156	LEU
1	B	1178	VAL
1	B	1188	VAL
1	B	1276	LEU
1	B	1279	GLU
1	B	1313	ARG
1	B	1375	ARG
1	B	1446	GLN
1	B	1507	SER
1	B	1513	ASN
1	B	1648	ARG
1	B	1667	GLN
1	B	1704	ILE
1	B	1742	THR
1	B	1777	SER
1	B	1788	LEU
1	B	1831	LEU
1	B	1840	THR
1	B	1858	ILE
1	B	1862	HIS
1	B	1863	HIS

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Mol	Chain	Res	Type
1	B	1864	GLU
1	B	1875	VAL
1	B	1879	LEU
1	B	1892	ASN
1	B	1910	SER
1	B	1979	VAL
1	B	1985	ILE
1	B	1997	LEU
1	B	2002	SER
1	B	2018	GLU
1	B	2040	GLN
1	B	2105	THR
2	J	2094	SER
2	J	2098	LYS
2	J	2099	GLU
2	J	2138	GLN
2	J	2170	LYS
2	J	2171	GLU
2	J	2173	GLU
2	J	2247	ASN
2	J	2287	ARG
2	J	2289	ASP

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	643	GLN
1	B	720	GLN
1	B	768	GLN
1	B	902	ASN
1	B	999	GLN
1	B	1003	GLN
1	B	1101	ASN
1	B	1502	HIS
1	B	1692	ASN
1	B	1892	ASN
1	B	2040	GLN
1	B	2058	GLN
1	B	2103	ASN
2	J	2155	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	A09	B	5801	-	9,11,11	2.68	3 (33%)	14,15,15	4.88	5 (35%)
4	EDO	B	5803	-	3,3,3	0.48	0	2,2,2	0.43	0
4	EDO	B	5810	-	3,3,3	0.54	0	2,2,2	0.65	0
4	EDO	B	5811	-	3,3,3	0.81	0	2,2,2	0.14	0
4	EDO	B	5805	-	3,3,3	0.49	0	2,2,2	0.30	0
4	EDO	B	5809	-	3,3,3	0.45	0	2,2,2	0.76	0
4	EDO	B	5808	-	3,3,3	0.53	0	2,2,2	0.43	0
4	EDO	B	5802	-	3,3,3	0.45	0	2,2,2	0.27	0
4	EDO	B	5807	-	3,3,3	0.77	0	2,2,2	0.47	0
4	EDO	B	5804	-	3,3,3	0.42	0	2,2,2	0.62	0
4	EDO	J	2401	-	3,3,3	0.51	0	2,2,2	0.42	0
4	EDO	B	5806	-	3,3,3	0.37	0	2,2,2	0.36	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	A09	B	5801	-	-	6/8/9/9	0/1/1/1
4	EDO	B	5803	-	-	0/1/1/1	-
4	EDO	B	5810	-	-	1/1/1/1	-
4	EDO	B	5811	-	-	1/1/1/1	-
4	EDO	B	5805	-	-	0/1/1/1	-
4	EDO	B	5809	-	-	1/1/1/1	-
4	EDO	B	5808	-	-	0/1/1/1	-
4	EDO	B	5802	-	-	1/1/1/1	-
4	EDO	B	5807	-	-	1/1/1/1	-
4	EDO	B	5804	-	-	0/1/1/1	-
4	EDO	J	2401	-	-	1/1/1/1	-
4	EDO	B	5806	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5801	A09	O2-S1	6.08	1.50	1.43
3	B	5801	A09	O1-S1	4.34	1.48	1.43
3	B	5801	A09	C1-S1	2.89	1.80	1.76

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5801	A09	O2-S1-O1	-14.91	101.42	119.52
3	B	5801	A09	O2-S1-N1	7.14	115.80	105.44
3	B	5801	A09	O1-S1-C1	5.53	114.96	107.98
3	B	5801	A09	O1-S1-N1	3.86	111.05	105.44
3	B	5801	A09	O2-S1-C1	-3.07	104.10	107.98

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5801	A09	O3-N1-S1-O1
3	B	5801	A09	O3-N1-S1-O2
3	B	5801	A09	C2-C1-S1-N1
3	B	5801	A09	C6-C1-S1-N1
3	B	5801	A09	C6-C1-S1-O2
3	B	5801	A09	C2-C1-S1-O2
4	B	5802	EDO	O1-C1-C2-O2
4	B	5806	EDO	O1-C1-C2-O2
4	J	2401	EDO	O1-C1-C2-O2

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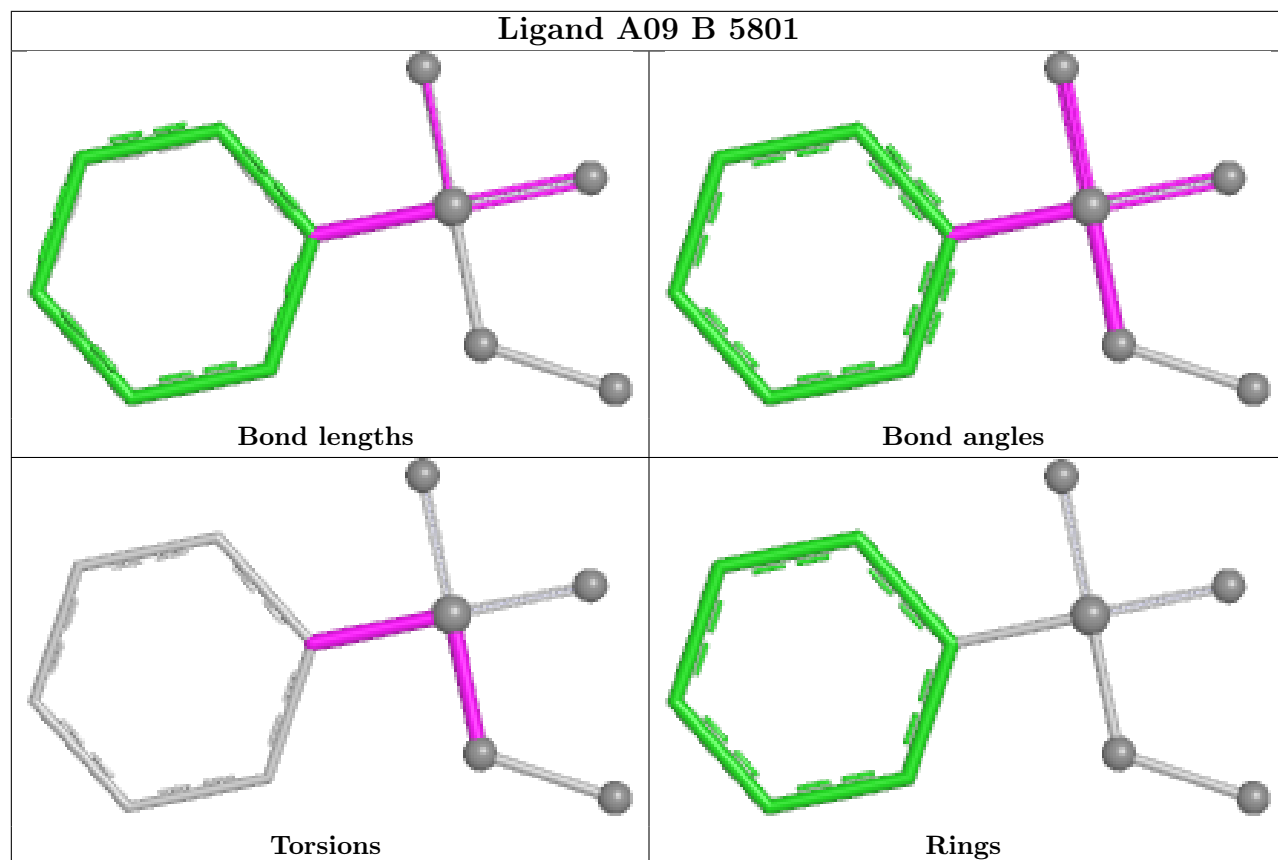
Mol	Chain	Res	Type	Atoms
4	B	5811	EDO	O1-C1-C2-O2
4	B	5807	EDO	O1-C1-C2-O2
4	B	5809	EDO	O1-C1-C2-O2
4	B	5810	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5802	EDO	2	0
4	B	5806	EDO	3	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	1724/1747 (98%)	0.26	65 (3%) 44 46	32, 61, 122, 189	0
2	J	263/263 (100%)	0.14	14 (5%) 32 34	39, 57, 121, 205	0
All	All	1987/2010 (98%)	0.25	79 (3%) 42 44	32, 60, 122, 205	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	ALA	5.7
1	B	575	LEU	5.7
1	B	1597	LEU	5.3
1	B	1860	ILE	4.9
2	J	2060	LEU	4.9
1	B	1601	LEU	4.6
1	B	1889	VAL	4.4
1	B	455	PHE	3.8
2	J	2063	MET	3.7
1	B	2038	LEU	3.4
1	B	1859	PRO	3.4
1	B	1997	LEU	3.3
1	B	1887	PRO	3.2
1	B	601	GLY	3.1
1	B	1868	LEU	3.0
1	B	1893	LEU	3.0
2	J	2062	SER	2.8
1	B	573	HIS	2.8
1	B	1858	ILE	2.8
1	B	405	PRO	2.8
1	B	1600	TYR	2.8
1	B	1879	LEU	2.8
1	B	812	THR	2.7
1	B	1416	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	580	ILE	2.7
1	B	1866	ASN	2.7
1	B	1614	LEU	2.7
2	J	2319	LEU	2.7
1	B	1857	ASN	2.6
1	B	1167	MET	2.6
2	J	2100	THR	2.6
1	B	454	PRO	2.6
1	B	778	LEU	2.5
1	B	1895	LEU	2.5
1	B	1861	ARG	2.5
1	B	726	HIS	2.5
1	B	2095	VAL	2.4
1	B	2127	LYS	2.4
2	J	2058	GLY	2.4
1	B	769	CYS	2.4
1	B	1598	ILE	2.4
1	B	1999	LEU	2.4
1	B	779	PRO	2.4
1	B	527	MET	2.4
2	J	2061	GLY	2.3
1	B	1872	ALA	2.3
2	J	2318	ALA	2.3
1	B	1884	PHE	2.3
1	B	1840	THR	2.3
1	B	1706	CYS	2.3
1	B	1995	ALA	2.3
2	J	2101	GLY	2.3
1	B	2002	SER	2.3
1	B	1873	GLN	2.2
2	J	2064	THR	2.2
1	B	1971	ILE	2.2
1	B	1908	LEU	2.2
1	B	603	ARG	2.2
1	B	1074	GLY	2.2
1	B	582	ALA	2.2
1	B	570	THR	2.2
1	B	605	TYR	2.1
2	J	2097	ILE	2.1
1	B	1325	PHE	2.1
1	B	1983	PHE	2.1
1	B	757	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	772	LEU	2.1
1	B	1584	ILE	2.1
2	J	2320	LEU	2.1
1	B	1891	THR	2.1
1	B	2026	LYS	2.1
1	B	2004	ILE	2.1
2	J	2220	PRO	2.1
1	B	1410	GLY	2.1
1	B	1978	GLY	2.1
2	J	2094	SER	2.1
1	B	2098	ALA	2.1
1	B	1604	LEU	2.1
1	B	1411	GLU	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.

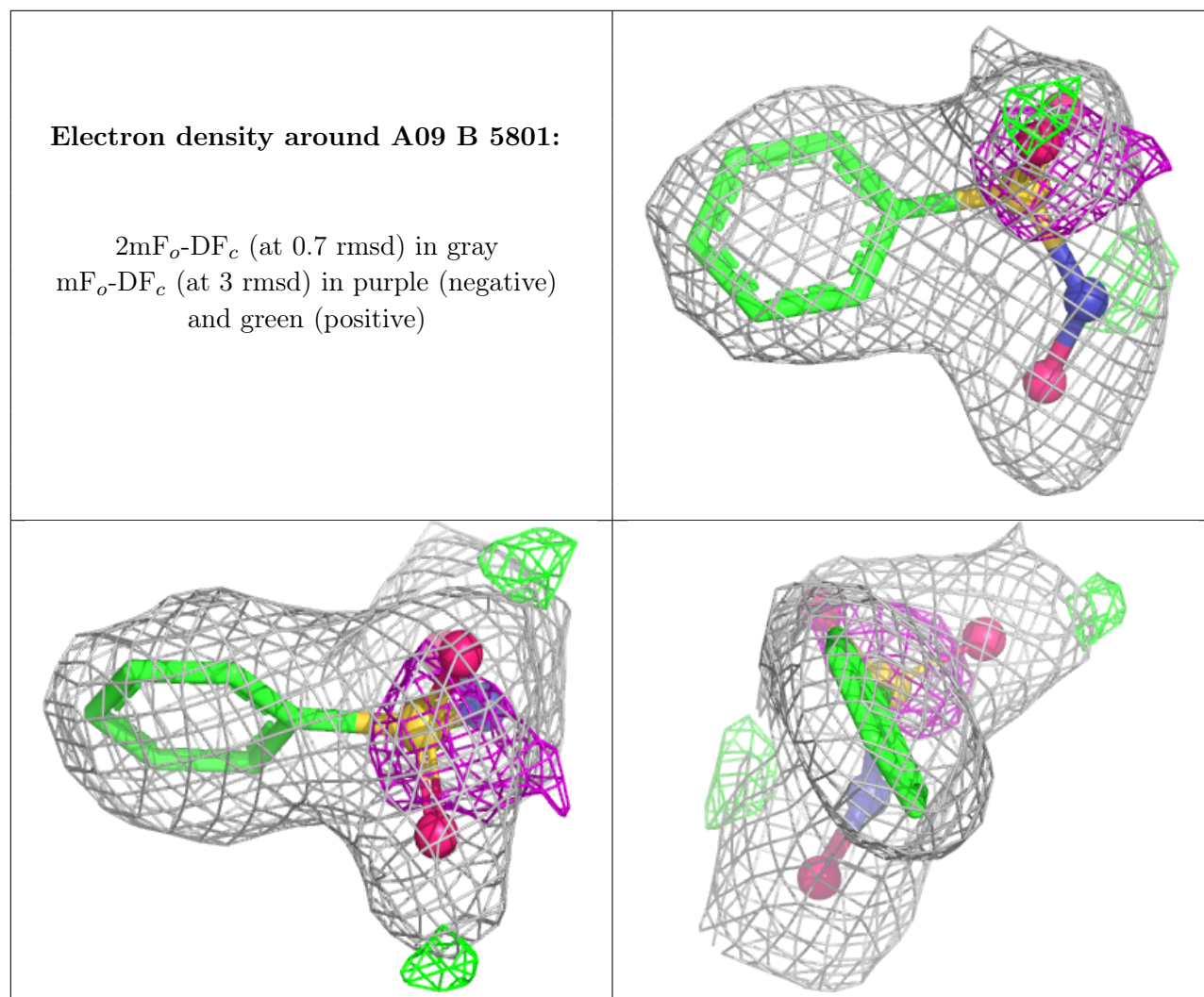
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	5803	4/4	0.64	0.18	56,63,68,71	0
4	EDO	B	5811	4/4	0.69	0.14	48,56,57,57	0
4	EDO	B	5804	4/4	0.72	0.17	58,60,61,69	0
4	EDO	J	2401	4/4	0.80	0.18	57,64,67,73	0
4	EDO	B	5805	4/4	0.82	0.17	56,56,59,65	0
4	EDO	B	5808	4/4	0.83	0.15	69,76,78,89	0
4	EDO	B	5810	4/4	0.85	0.16	60,63,65,68	0
4	EDO	B	5806	4/4	0.86	0.15	50,53,59,64	0
3	A09	B	5801	11/11	0.88	0.11	44,50,61,67	0
4	EDO	B	5809	4/4	0.91	0.12	43,49,60,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	5807	4/4	0.91	0.11	41,42,43,45	0
4	EDO	B	5802	4/4	0.92	0.12	36,51,61,64	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.