



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:13 AM UTC

PDB ID : 7BDL / pdb_00007bdl
Title : Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and mant-ADP
Authors : Vester, K.; Santos, K.F.; Absmeier, E.; Wahl, M.C.
Deposited on : 2020-12-21
Resolution : 2.69 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

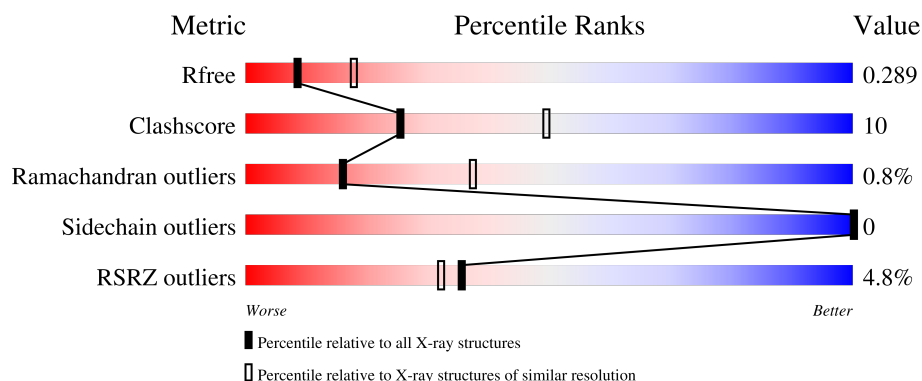
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	5% 76% 22% .
2	J	263	3% 84% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16356 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	1725	Total	C	N	O	S	0	0	0
			13870	8865	2373	2560	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

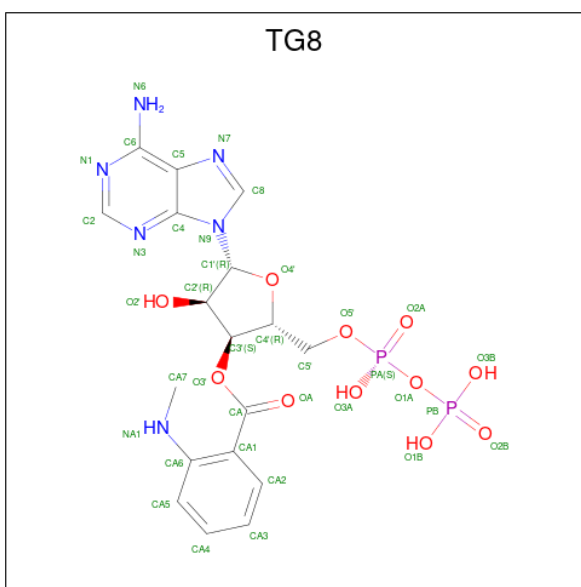
- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	262	Total	C	N	O	S	0	0	0
			2118	1356	364	386	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 [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-2-[[oxidanyl(phosphonooxy)phosphoryl]oxymethyl]oxolan-3-yl] 2-(methylamino)benzoate (CCD ID: TG8) (formula: C₁₈H₂₂N₆O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



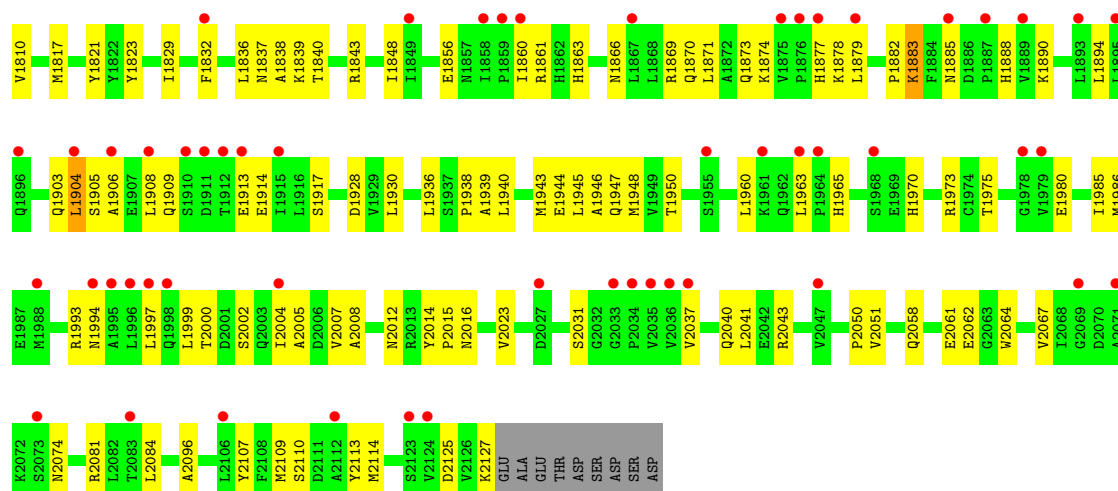
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 37	C 18	N 6	O 11	P 2	0	0
3	B	1	Total 37	C 18	N 6	O 11	P 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

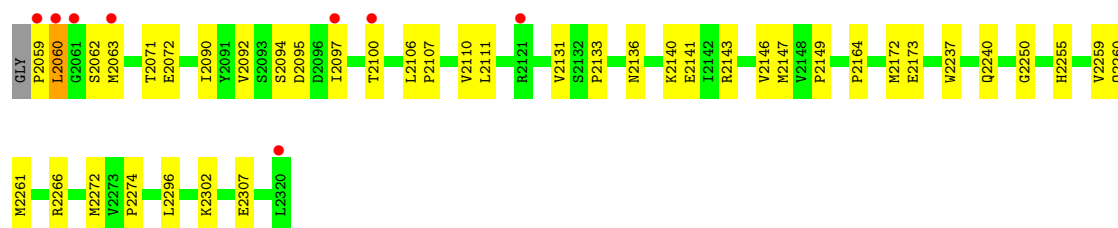
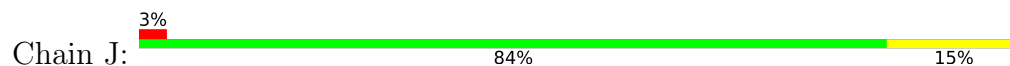
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Mg 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	263	Total O 263 263	0	0
5	J	29	Total O 29 29	0	0



● 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	99.93Å 118.78Å 187.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.44 – 2.69 48.44 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.44-2.69) 99.4 (48.44-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.232 , 0.292 0.233 , 0.289	Depositor DCC
R_{free} test set	2100 reflections (3.35%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 24.8	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	0.92	EDS
Total number of atoms	16356	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: TG8, MG

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	0.12	0/14164	0.30	1/19191 (0.0%)
2	J	0.10	0/2185	0.32	0/2975
All	All	0.12	0/16349	0.31	1/22166 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	LYS	CB-CG-CD	-6.01	97.47	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	2060	LEU	Peptide

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	13870	0	14018	282	0
2	J	2118	0	2061	27	0
3	B	74	0	0	0	0
4	B	2	0	0	0	0
5	B	263	0	0	13	0
5	J	29	0	0	1	0
All	All	16356	0	16079	307	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 10.

All (307) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:THR:HG23	1:B:579:GLU:OE2	1.31	1.28
1:B:1482:GLU:OE1	1:B:1483:ARG:HG2	1.68	0.94
1:B:570:THR:CG2	1:B:579:GLU:OE2	2.22	0.83
1:B:1456:VAL:HG12	1:B:1491:SER:HB2	1.63	0.79
1:B:2043:ARG:NH1	1:B:2062:GLU:OE1	2.17	0.78
1:B:1141:LYS:HA	1:B:1144:GLU:HB2	1.68	0.75
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.69	0.73
1:B:1136:PRO:HB2	1:B:1138:GLU:OE2	1.90	0.70
1:B:1905:SER:HB3	1:B:1908:LEU:HB3	1.72	0.70
1:B:1871:LEU:HD12	1:B:1874:LYS:HB2	1.74	0.70
1:B:1997:LEU:HB3	1:B:1999:LEU:CD1	2.22	0.69
1:B:2023:VAL:HG13	1:B:2037:VAL:HG22	1.75	0.69
1:B:1843:ARG:NE	1:B:1877:HIS:HB3	2.09	0.67
1:B:1843:ARG:HE	1:B:1877:HIS:HB3	1.60	0.67
1:B:1138:GLU:HB3	1:B:1139:VAL:HG23	1.77	0.65
1:B:1838:ALA:O	1:B:2074:ASN:ND2	2.29	0.65
1:B:893:MET:HG2	1:B:900:MET:HE1	1.78	0.65
1:B:1894:LEU:HD11	1:B:1908:LEU:HD21	1.77	0.65
1:B:971:LYS:HB2	1:B:980:GLN:HB3	1.79	0.65
1:B:421:HIS:ND1	5:B:2306:HOH:O	2.30	0.65
1:B:1152:ARG:HH11	1:B:1164:LEU:HD11	1.62	0.64
1:B:469:LYS:HA	1:B:472:GLN:HG3	1.79	0.64
1:B:526:ASN:H	1:B:531:ILE:HG22	1.62	0.64
1:B:1997:LEU:HB3	1:B:1999:LEU:HD13	1.81	0.63
1:B:1413:SER:HB2	1:B:2061:GLU:HB2	1.81	0.62
1:B:570:THR:OG1	1:B:573:HIS:ND1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1648:ARG:NH1	5:B:2307:HOH:O	2.31	0.62
2:J:2140:LYS:NZ	2:J:2173:GLU:OE2	2.28	0.62
1:B:1667:GLN:NE2	5:B:2309:HOH:O	2.31	0.61
1:B:1598:ILE:HD12	1:B:1598:ILE:H	1.66	0.61
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.82	0.61
1:B:1339:VAL:HA	1:B:1486:ARG:HH22	1.65	0.60
1:B:1696:GLN:NE2	5:B:2311:HOH:O	2.33	0.60
1:B:444:GLU:HG2	1:B:690:VAL:HG22	1.83	0.60
2:J:2133:PRO:HG2	2:J:2136:ASN:HB3	1.83	0.60
1:B:547:LEU:HG	1:B:551:MET:HE2	1.84	0.60
1:B:1829:ILE:HA	1:B:1832:PHE:HB2	1.83	0.60
1:B:1314:ASN:HB3	1:B:1317:PHE:HB2	1.84	0.60
1:B:1415:ASP:HB3	1:B:1435:LEU:HD11	1.83	0.60
1:B:513:ALA:HB1	1:B:613:ILE:HD13	1.84	0.60
1:B:1436:SER:HA	1:B:1445:VAL:HG11	1.84	0.59
1:B:604:THR:OG1	1:B:605:TYR:N	2.34	0.59
1:B:1195:ARG:HD3	1:B:1260:GLU:OE2	2.03	0.59
1:B:2000:THR:HG22	1:B:2002:SER:H	1.66	0.58
1:B:993:ILE:HD12	1:B:1091:LEU:HD23	1.85	0.58
1:B:602:GLU:HA	1:B:604:THR:HG22	1.85	0.58
1:B:1943:MET:HE3	1:B:2109:MET:HE3	1.85	0.58
1:B:1997:LEU:C	1:B:1999:LEU:HD12	2.29	0.57
2:J:2141:GLU:OE2	2:J:2143:ARG:NH2	2.37	0.57
2:J:2146:VAL:HG22	2:J:2272:MET:HB2	1.85	0.57
1:B:756:SER:OG	1:B:757:ALA:N	2.36	0.57
1:B:1302:LEU:N	1:B:1334:GLN:OE1	2.38	0.57
1:B:1271:VAL:HG22	1:B:1279:GLU:HG3	1.86	0.57
2:J:2090:ILE:HG21	2:J:2111:LEU:HD21	1.86	0.57
1:B:1395:GLU:HA	1:B:1399:ASP:HB2	1.86	0.57
1:B:1575:ASP:O	1:B:1579:THR:HG22	2.04	0.57
1:B:2043:ARG:HB2	1:B:2084:LEU:HD21	1.87	0.56
1:B:1741:VAL:HG13	1:B:1817:MET:HG2	1.87	0.56
1:B:1124:GLN:N	2:J:2307:GLU:OE2	2.37	0.56
1:B:1139:VAL:O	1:B:1142:LYS:HB3	2.06	0.56
1:B:1986:MET:HG2	1:B:1993:ARG:HH12	1.69	0.56
1:B:1438:ARG:NH1	1:B:1821:TYR:O	2.39	0.55
1:B:1375:ARG:NH2	1:B:1419:LEU:O	2.39	0.55
1:B:1604:LEU:HD12	1:B:1610:LYS:HG2	1.87	0.55
1:B:473:ALA:O	1:B:476:GLU:HG3	2.07	0.55
1:B:654:THR:HG21	1:B:677:ASP:HA	1.88	0.55
1:B:1187:SER:HB3	1:B:1203:THR:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1482:GLU:HG2	1:B:1483:ARG:NE	2.22	0.55
1:B:1986:MET:HA	1:B:1993:ARG:CZ	2.37	0.55
1:B:1570:ARG:NH1	5:B:2301:HOH:O	2.20	0.55
1:B:1729:ASP:OD1	1:B:1729:ASP:N	2.40	0.55
1:B:1194:THR:HG23	1:B:1196:SER:H	1.71	0.55
1:B:1475:ARG:HD3	1:B:1504:LEU:HA	1.88	0.55
1:B:790:THR:HG22	1:B:792:VAL:H	1.72	0.54
1:B:1122:MET:HE2	1:B:1276:LEU:HD23	1.88	0.54
2:J:2302:LYS:NZ	5:J:2404:HOH:O	2.39	0.54
1:B:1753:ASP:O	1:B:1756:THR:OG1	2.26	0.54
1:B:1860:ILE:HG12	1:B:1885:ASN:OD1	2.07	0.54
1:B:1298:PRO:HB3	1:B:1515:HIS:CG	2.43	0.54
1:B:1606:ASP:OD1	1:B:1607:SER:N	2.40	0.54
1:B:495:THR:HG22	1:B:497:GLU:H	1.73	0.54
1:B:1468:GLU:OE1	1:B:1760:LEU:N	2.38	0.54
1:B:1472:SER:OG	1:B:1503:TRP:NE1	2.36	0.54
1:B:1843:ARG:HD3	1:B:1877:HIS:HD2	1.73	0.53
1:B:1986:MET:HA	1:B:1993:ARG:NH2	2.24	0.53
1:B:740:ASP:HA	1:B:743:LEU:HD12	1.91	0.53
1:B:1515:HIS:CE1	1:B:1721:PRO:HG3	2.44	0.53
1:B:580:ILE:HG23	1:B:586:ILE:HD11	1.91	0.53
1:B:926:TYR:HA	1:B:929:MET:HE2	1.90	0.53
1:B:1604:LEU:HB2	1:B:1610:LYS:HE3	1.91	0.53
1:B:1139:VAL:HG13	1:B:1142:LYS:HE2	1.91	0.53
2:J:2250:GLY:O	2:J:2255:HIS:NE2	2.41	0.53
1:B:1325:PHE:HB3	1:B:1695:LEU:HD11	1.91	0.53
1:B:545:ARG:H	1:B:545:ARG:HD3	1.73	0.53
1:B:1879:LEU:HD23	1:B:1879:LEU:H	1.73	0.53
1:B:1840:THR:HB	1:B:1938:PRO:HB3	1.91	0.52
1:B:533:VAL:HB	1:B:584:GLN:HG2	1.91	0.52
1:B:1773:LEU:HD21	1:B:1784:HIS:HB2	1.91	0.52
2:J:2131:VAL:HG13	2:J:2172:MET:HG2	1.91	0.52
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	1.90	0.52
1:B:1304:LEU:HD12	1:B:1334:GLN:HG2	1.92	0.52
1:B:525:ILE:HA	1:B:531:ILE:HB	1.91	0.52
1:B:537:LYS:NZ	5:B:2322:HOH:O	2.43	0.52
1:B:1997:LEU:O	1:B:1999:LEU:HD12	2.10	0.52
2:J:2100:THR:OG1	2:J:2259:VAL:HG12	2.10	0.52
2:J:2106:LEU:HD12	2:J:2107:PRO:HD2	1.93	0.51
1:B:1960:LEU:HD23	1:B:1985:ILE:HD11	1.93	0.51
1:B:1856:GLU:OE2	1:B:1888:HIS:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1284:VAL:O	1:B:1284:VAL:HG23	2.10	0.50
1:B:1577:LEU:HD11	1:B:1612:THR:HA	1.94	0.50
1:B:1936:LEU:HB3	1:B:2074:ASN:HA	1.93	0.50
1:B:763:ARG:NH2	1:B:764:THR:OG1	2.44	0.50
1:B:579:GLU:O	1:B:583:THR:HG23	2.11	0.50
1:B:404:ALA:O	1:B:406:ARG:NH1	2.45	0.50
1:B:1778:HIS:HA	1:B:1781:LEU:HD12	1.94	0.50
1:B:1947:GLN:HG3	1:B:2114:MET:HG2	1.94	0.50
1:B:1024:PHE:HB3	1:B:1027:ILE:HD12	1.92	0.50
1:B:1417:LYS:NZ	5:B:2318:HOH:O	2.41	0.50
1:B:1693:ARG:HD3	1:B:1697:ASP:OD2	2.11	0.50
1:B:1866:ASN:HA	1:B:1869:ARG:HB2	1.93	0.50
1:B:1960:LEU:HD11	1:B:1980:GLU:HA	1.94	0.50
1:B:1970:HIS:HB2	1:B:1973:ARG:HB2	1.93	0.50
1:B:752:LEU:HD11	1:B:762:LEU:HD12	1.94	0.50
1:B:575:LEU:C	1:B:577:LYS:H	2.20	0.49
1:B:1481:ILE:HG13	1:B:1482:GLU:H	1.78	0.49
2:J:2071:THR:HG22	2:J:2072:GLU:OE2	2.12	0.49
1:B:1210:TRP:HA	1:B:1215:HIS:CD2	2.48	0.49
1:B:1608:THR:HG22	1:B:1612:THR:HG23	1.93	0.49
1:B:671:LYS:NZ	5:B:2326:HOH:O	2.46	0.49
1:B:1963:LEU:HD13	1:B:2007:VAL:HG13	1.95	0.49
1:B:457:SER:OG	1:B:458:GLU:N	2.37	0.48
1:B:704:MET:HG3	1:B:870:ILE:HG21	1.96	0.48
1:B:1210:TRP:HA	1:B:1215:HIS:HD2	1.77	0.48
1:B:1837:ASN:OD1	1:B:1839:LYS:HG2	2.13	0.48
1:B:828:ILE:HD12	1:B:869:LEU:HD12	1.95	0.48
1:B:1328:PHE:HB3	1:B:1332:GLN:HB2	1.96	0.48
1:B:1430:GLU:HG2	1:B:1466:VAL:HG11	1.96	0.48
1:B:1878:LYS:HE3	1:B:1878:LYS:HB3	1.58	0.48
1:B:812:THR:OG1	1:B:813:ALA:N	2.46	0.48
1:B:1946:ALA:O	1:B:1950:THR:OG1	2.25	0.48
1:B:1123:TRP:HB3	2:J:2307:GLU:OE2	2.13	0.48
1:B:1412:THR:O	1:B:1416:LEU:HD12	2.14	0.48
1:B:1836:LEU:HG	1:B:1848:ILE:HD13	1.94	0.48
1:B:1574:ILE:HD11	1:B:1608:THR:HG21	1.96	0.48
1:B:603:ARG:NH2	1:B:1676:TYR:OH	2.47	0.48
1:B:1843:ARG:HD2	1:B:1843:ARG:HA	1.57	0.48
1:B:1945:LEU:HA	1:B:1948:MET:HB2	1.96	0.48
1:B:1607:SER:OG	1:B:1608:THR:N	2.47	0.48
1:B:1598:ILE:HA	1:B:1601:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:PRO:HG2	1:B:466:LYS:HG2	1.96	0.47
1:B:756:SER:HB3	1:B:759:THR:OG1	2.14	0.47
1:B:1170:MET:HB3	1:B:1173:THR:HB	1.96	0.47
1:B:1663:ILE:HD12	1:B:1704:ILE:HG12	1.95	0.47
1:B:403:LEU:N	5:B:2324:HOH:O	2.46	0.47
1:B:639:ILE:O	1:B:643:GLN:N	2.32	0.47
1:B:1356:LYS:NZ	5:B:2325:HOH:O	2.47	0.47
1:B:2114:MET:HE2	1:B:2114:MET:HB3	1.85	0.47
1:B:1190:LEU:HD22	1:B:1198:LEU:HD21	1.96	0.47
1:B:626:PRO:HG3	1:B:893:MET:HA	1.95	0.47
1:B:2051:VAL:HG13	1:B:2113:TYR:CZ	2.50	0.47
1:B:525:ILE:HG22	1:B:531:ILE:HG12	1.97	0.47
1:B:785:HIS:CE1	1:B:794:ARG:HD2	2.50	0.47
1:B:1298:PRO:HB3	1:B:1515:HIS:CD2	2.50	0.47
1:B:529:GLY:O	1:B:531:ILE:HG23	2.15	0.47
1:B:1381:PRO:HB2	1:B:1458:LEU:HD12	1.97	0.47
1:B:2008:ALA:O	1:B:2012:ASN:ND2	2.30	0.47
2:J:2059:PRO:HG2	2:J:2060:LEU:H	1.79	0.47
1:B:994:THR:HG22	1:B:1023:GLU:OE2	2.15	0.46
1:B:545:ARG:HD3	1:B:545:ARG:N	2.30	0.46
1:B:777:LEU:HB3	1:B:782:PHE:HB2	1.98	0.46
1:B:1434:ILE:HD13	1:B:1823:TYR:HB2	1.96	0.46
1:B:1965:HIS:O	1:B:1999:LEU:HD21	2.16	0.46
2:J:2141:GLU:OE1	2:J:2266:ARG:NH2	2.48	0.46
1:B:566:VAL:HG22	1:B:585:ILE:HB	1.98	0.46
1:B:1482:GLU:HG2	1:B:1483:ARG:HE	1.80	0.46
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	1.96	0.46
1:B:1579:THR:O	1:B:1583:ASP:OD1	2.34	0.46
1:B:766:ALA:O	1:B:775:LYS:NZ	2.40	0.46
1:B:1287:ARG:NH2	5:B:2328:HOH:O	2.48	0.46
2:J:2237:TRP:O	2:J:2240:GLN:HG3	2.16	0.46
1:B:858:ARG:C	1:B:860:GLN:H	2.23	0.46
1:B:1903:GLN:HG2	1:B:1904:LEU:H	1.80	0.46
1:B:1905:SER:O	1:B:1908:LEU:N	2.48	0.46
1:B:1072:LEU:H	1:B:1078:MET:HE3	1.81	0.46
1:B:1136:PRO:HB2	1:B:1138:GLU:CD	2.41	0.46
1:B:1600:TYR:HB3	1:B:1631:LEU:HD12	1.98	0.46
1:B:526:ASN:H	1:B:531:ILE:CG2	2.28	0.45
1:B:602:GLU:C	1:B:604:THR:H	2.22	0.45
1:B:677:ASP:HB2	1:B:885:GLN:HE22	1.82	0.45
1:B:1456:VAL:O	1:B:1459:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2092:VAL:HG13	2:J:2261:MET:HE3	1.98	0.45
1:B:758:SER:OG	1:B:805:HIS:ND1	2.45	0.45
1:B:1871:LEU:HA	1:B:1874:LYS:HG3	1.98	0.45
1:B:1871:LEU:HA	1:B:1874:LYS:HB2	1.98	0.45
1:B:581:SER:HB3	1:B:605:TYR:CZ	2.51	0.45
1:B:2064:TRP:CZ3	1:B:2110:SER:HB3	2.52	0.45
1:B:1883:LYS:HZ1	1:B:1885:ASN:H	1.65	0.45
2:J:2149:PRO:HD3	2:J:2274:PRO:HG3	1.97	0.45
1:B:1482:GLU:O	1:B:1483:ARG:HD3	2.17	0.45
2:J:2063:MET:HE3	2:J:2063:MET:HB3	1.85	0.45
1:B:1760:LEU:O	1:B:1764:MET:HG3	2.17	0.45
1:B:1843:ARG:HA	1:B:1843:ARG:HH21	1.82	0.45
1:B:1944:GLU:HA	1:B:1947:GLN:HG2	1.99	0.45
1:B:1335:VAL:O	1:B:1339:VAL:HG23	2.17	0.45
1:B:811:SER:OG	1:B:812:THR:N	2.50	0.44
1:B:1566:ARG:HG3	1:B:1621:HIS:CG	2.53	0.44
1:B:1183:LYS:HE3	1:B:1207:ASP:HB3	1.99	0.44
1:B:1930:LEU:HD13	1:B:1938:PRO:HB2	2.00	0.44
1:B:1262:LEU:HA	1:B:1263:PRO:HD3	1.90	0.44
1:B:1475:ARG:NH1	1:B:1504:LEU:O	2.50	0.44
1:B:984:LEU:HD21	1:B:1002:ASN:HB2	1.98	0.44
1:B:1562:PHE:HE1	1:B:1654:MET:HE1	1.83	0.44
1:B:1939:ALA:O	1:B:1943:MET:HG3	2.18	0.44
2:J:2071:THR:HG22	2:J:2072:GLU:H	1.83	0.44
1:B:426:LYS:HD3	1:B:426:LYS:N	2.32	0.44
1:B:1313:ARG:HA	1:B:1313:ARG:HD3	1.82	0.44
1:B:1395:GLU:OE1	1:B:1400:ARG:NH1	2.51	0.44
1:B:1914:GLU:O	1:B:1917:SER:OG	2.30	0.44
1:B:2014:TYR:O	1:B:2016:ASN:N	2.50	0.44
1:B:2067:VAL:HB	1:B:2107:TYR:HB2	1.99	0.44
1:B:525:ILE:HG22	1:B:531:ILE:HG21	2.00	0.44
1:B:790:THR:HG22	1:B:792:VAL:N	2.33	0.44
1:B:1663:ILE:HD13	1:B:1687:MET:HE3	1.98	0.44
1:B:1123:TRP:HD1	1:B:1126:MET:HE3	1.83	0.44
1:B:1483:ARG:HD3	1:B:1483:ARG:HA	1.78	0.43
1:B:1837:ASN:ND2	1:B:1840:THR:OG1	2.51	0.43
1:B:421:HIS:NE2	1:B:875:GLU:OE1	2.32	0.43
1:B:492:ALA:HA	1:B:647:ARG:HH22	1.83	0.43
1:B:1195:ARG:NH1	1:B:1260:GLU:OE2	2.51	0.43
1:B:1383:GLU:OE2	1:B:1431:LYS:NZ	2.39	0.43
2:J:2062:SER:O	2:J:2062:SER:OG	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:ASP:O	1:B:797:VAL:HG23	2.19	0.43
1:B:1140:VAL:HA	1:B:1143:ILE:HD12	2.00	0.43
2:J:2107:PRO:HG2	2:J:2110:VAL:HG22	1.99	0.43
1:B:1199:LYS:NZ	5:B:2333:HOH:O	2.51	0.43
1:B:785:HIS:HB3	1:B:811:SER:HB2	2.00	0.43
1:B:436:ARG:HG2	1:B:445:VAL:HG22	2.01	0.43
1:B:1194:THR:OG1	1:B:1195:ARG:N	2.51	0.43
1:B:1908:LEU:HD23	1:B:1908:LEU:O	2.19	0.43
1:B:1870:GLN:O	1:B:1873:GLN:HG2	2.19	0.42
1:B:2040:GLN:O	1:B:2041:LEU:HD13	2.19	0.42
1:B:416:PHE:HB2	1:B:892:GLN:OE1	2.19	0.42
1:B:1456:VAL:CG1	1:B:1491:SER:HB2	2.43	0.42
1:B:1483:ARG:HB3	1:B:1484:PRO:HD2	2.00	0.42
1:B:711:LYS:HD3	1:B:868:ILE:HG21	2.01	0.42
1:B:1761:TYR:CE1	1:B:1785:LEU:HD11	2.54	0.42
1:B:754:GLU:O	1:B:756:SER:N	2.49	0.42
1:B:2125:ASP:O	1:B:2127:LYS:NZ	2.47	0.42
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.54	0.42
1:B:1159:ASN:OD1	1:B:1159:ASN:N	2.48	0.42
1:B:1917:SER:HA	1:B:2058:GLN:NE2	2.34	0.42
1:B:690:VAL:HG11	1:B:707:ILE:HD13	2.01	0.42
1:B:1861:ARG:HB3	1:B:1863:HIS:CD2	2.55	0.42
1:B:1890:LYS:HE3	1:B:1890:LYS:HB2	1.89	0.42
2:J:2164:PRO:HB3	2:J:2296:LEU:HD11	2.02	0.42
1:B:1499:ASP:OD2	1:B:1763:ARG:NH1	2.47	0.42
1:B:1503:TRP:CD2	1:B:1759:PHE:HB2	2.54	0.42
1:B:721:VAL:HG22	1:B:825:THR:HB	2.02	0.42
1:B:1259:PHE:CZ	1:B:1263:PRO:HG3	2.54	0.42
1:B:1457:HIS:HB3	1:B:1491:SER:OG	2.20	0.42
2:J:2147:MET:O	2:J:2274:PRO:HD3	2.19	0.42
1:B:1843:ARG:HD3	1:B:1877:HIS:CD2	2.52	0.42
1:B:1909:GLN:NE2	1:B:1913:GLU:OE2	2.53	0.42
1:B:778:LEU:HD23	1:B:778:LEU:HA	1.93	0.42
1:B:579:GLU:H	1:B:579:GLU:HG3	1.67	0.41
1:B:460:GLN:N	1:B:460:GLN:OE1	2.53	0.41
1:B:570:THR:N	1:B:579:GLU:OE2	2.53	0.41
1:B:622:ASP:OD1	1:B:623:ASP:N	2.53	0.41
1:B:1167:MET:HG2	1:B:1169:LYS:H	1.85	0.41
2:J:2060:LEU:HA	2:J:2062:SER:HB3	2.03	0.41
1:B:1894:LEU:HD21	1:B:1908:LEU:HD21	2.02	0.41
1:B:742:CYS:O	1:B:746:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1515:HIS:HB3	1:B:1516:PRO:HD2	2.02	0.41
1:B:1994:ASN:O	1:B:1994:ASN:ND2	2.54	0.41
2:J:2100:THR:H	2:J:2260:GLN:HE22	1.67	0.41
1:B:1732:MET:HE3	1:B:1788:LEU:HD21	2.02	0.41
1:B:1936:LEU:O	1:B:1940:LEU:HG	2.20	0.41
1:B:1167:MET:SD	1:B:1170:MET:N	2.92	0.41
1:B:1417:LYS:HA	1:B:1417:LYS:HD3	1.70	0.41
1:B:574:GLN:O	5:B:2302:HOH:O	2.21	0.41
1:B:666:ARG:HH11	1:B:922:TYR:HE1	1.67	0.41
1:B:1559:VAL:HG22	1:B:1660:LEU:HB3	2.03	0.41
1:B:762:LEU:HD23	1:B:762:LEU:HA	1.92	0.41
1:B:827:ILE:HG12	1:B:868:ILE:HB	2.03	0.41
1:B:1307:LEU:CB	1:B:1333:THR:HG22	2.51	0.41
1:B:1515:HIS:O	1:B:1518:VAL:HG22	2.20	0.41
1:B:1928:ASP:OD1	1:B:2081:ARG:NH1	2.53	0.41
1:B:2004:ILE:HD12	1:B:2005:ALA:N	2.35	0.41
2:J:2094:SER:HB2	2:J:2095:ASP:H	1.72	0.41
1:B:1009:LEU:HD11	1:B:1013:GLU:HG2	2.02	0.41
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.61	0.41
1:B:1347:PHE:CE2	1:B:1497:ALA:HB1	2.56	0.41
1:B:551:MET:HA	1:B:554:SER:HB3	2.03	0.40
1:B:1040:LEU:O	1:B:1044:VAL:HG13	2.22	0.40
1:B:1606:ASP:HB3	1:B:1609:LEU:HB3	2.04	0.40
1:B:1986:MET:HA	1:B:1993:ARG:NH1	2.36	0.40
1:B:513:ALA:HB2	1:B:651:LEU:HD11	2.02	0.40
1:B:702:GLN:HA	1:B:705:ASN:HB2	2.03	0.40
1:B:1338:THR:O	1:B:1342:SER:HB3	2.21	0.40
1:B:1993:ARG:O	1:B:1997:LEU:HD12	2.21	0.40
1:B:849:ILE:HG13	1:B:879:TYR:HE1	1.87	0.40
1:B:935:LEU:HD23	1:B:935:LEU:HA	1.97	0.40
1:B:1804:ILE:HG12	1:B:1810:VAL:HG12	2.04	0.40
1:B:2031:SER:HA	1:B:2096:ALA:HB3	2.03	0.40
1:B:652:SER:OG	1:B:653:ALA:O	2.39	0.40
1:B:964:LEU:HB3	1:B:970:VAL:HG23	2.03	0.40
1:B:967:ASN:HB3	1:B:999:GLN:HB2	2.03	0.40

There are no symmetry-related clashes.

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	1723/1747 (99%)	1615 (94%)	93 (5%)	15 (1%)	14	35
2	J	260/263 (99%)	244 (94%)	15 (6%)	1 (0%)	30	54
All	All	1983/2010 (99%)	1859 (94%)	108 (5%)	16 (1%)	16	37

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1138	GLU
1	B	1882	PRO
1	B	1975	THR
1	B	455	PHE
1	B	457	SER
1	B	1883	LYS
1	B	2050	PRO
1	B	604	THR
1	B	1482	GLU
1	B	1904	LEU
1	B	2015	PRO
1	B	755	GLY
1	B	1906	ALA
1	B	576	CYS
1	B	1260	GLU
2	J	2097	ILE

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	1544/1560 (99%)	1544 (100%)	0	100	100
2	J	236/236 (100%)	236 (100%)	0	100	100
All	All	1780/1796 (99%)	1780 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	485	GLN
1	B	820	ASN
1	B	1026	ASN
1	B	1101	ASN
1	B	1124	GLN
1	B	1157	ASN
1	B	1189	HIS
1	B	1191	GLN
1	B	1215	HIS
1	B	1370	GLN
1	B	1402	ASN
1	B	1423	ASN
1	B	1441	GLN
1	B	1568	GLN
1	B	1615	ASN
1	B	1707	GLN
1	B	1873	GLN
1	B	1924	GLN
1	B	1947	GLN
2	J	2155	GLN
2	J	2158	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	TG8	B	2202	4	39,40,40	3.42	19 (48%)	58,60,60	2.09	13 (22%)
3	TG8	B	2201	4	39,40,40	3.44	19 (48%)	58,60,60	2.24	15 (25%)

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	TG8	B	2202	4	-	6/26/42/42	0/4/4/4
3	TG8	B	2201	4	-	8/26/42/42	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2201	TG8	CA2-CA1	8.80	1.53	1.39
3	B	2202	TG8	CA2-CA1	8.71	1.53	1.39
3	B	2201	TG8	CA5-CA6	8.25	1.53	1.39
3	B	2202	TG8	CA5-CA6	8.20	1.53	1.39
3	B	2202	TG8	CA3-CA4	6.78	1.53	1.38
3	B	2201	TG8	CA3-CA4	6.75	1.53	1.38
3	B	2202	TG8	CA1-CA6	-5.76	1.32	1.41
3	B	2201	TG8	CA1-CA6	-5.69	1.32	1.41
3	B	2201	TG8	PA-O1A	5.54	1.65	1.59
3	B	2202	TG8	PA-O1A	5.31	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2202	TG8	C6-N6	4.48	1.45	1.34
3	B	2201	TG8	C6-N6	4.41	1.45	1.34
3	B	2201	TG8	CA6-NA1	4.38	1.45	1.37
3	B	2202	TG8	CA6-NA1	4.37	1.45	1.37
3	B	2202	TG8	C5-N7	4.28	1.46	1.39
3	B	2201	TG8	C5-N7	4.20	1.46	1.39
3	B	2202	TG8	O4'-C1'	4.15	1.51	1.42
3	B	2202	TG8	CA3-CA2	-4.08	1.31	1.38
3	B	2201	TG8	CA3-CA2	-4.07	1.31	1.38
3	B	2201	TG8	O4'-C1'	4.04	1.51	1.42
3	B	2201	TG8	CA4-CA5	-3.96	1.32	1.38
3	B	2202	TG8	CA4-CA5	-3.95	1.32	1.38
3	B	2202	TG8	C2'-C3'	-3.71	1.44	1.53
3	B	2201	TG8	C2'-C3'	-3.48	1.45	1.53
3	B	2202	TG8	C8-N7	3.35	1.38	1.31
3	B	2201	TG8	C8-N7	3.33	1.38	1.31
3	B	2201	TG8	O4'-C4'	3.17	1.52	1.45
3	B	2201	TG8	O3'-CA	3.10	1.41	1.34
3	B	2202	TG8	O3'-CA	2.84	1.40	1.34
3	B	2202	TG8	O4'-C4'	2.78	1.51	1.45
3	B	2202	TG8	C4-N9	-2.40	1.32	1.37
3	B	2201	TG8	C4-N9	-2.36	1.32	1.37
3	B	2202	TG8	PB-O3B	-2.23	1.46	1.54
3	B	2201	TG8	PB-O3B	-2.22	1.46	1.54
3	B	2201	TG8	PB-O1B	-2.21	1.46	1.54
3	B	2202	TG8	PB-O1B	-2.21	1.46	1.54
3	B	2201	TG8	C5-C6	-2.06	1.35	1.41
3	B	2202	TG8	C5-C6	-2.02	1.35	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2201	TG8	C4-N9-C8	8.11	114.25	105.74
3	B	2202	TG8	C4-N9-C8	8.02	114.16	105.74
3	B	2201	TG8	N9-C8-N7	-5.33	106.37	113.94
3	B	2201	TG8	N1-C2-N3	-5.24	120.65	128.58
3	B	2202	TG8	N1-C2-N3	-5.22	120.67	128.58
3	B	2202	TG8	N9-C8-N7	-5.20	106.56	113.94
3	B	2201	TG8	O3'-CA-CA1	5.03	119.71	111.71
3	B	2202	TG8	O3'-CA-CA1	4.27	118.51	111.71
3	B	2201	TG8	C5-C4-N3	-3.84	121.43	126.72
3	B	2201	TG8	C4'-O4'-C1'	-3.82	101.02	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2202	TG8	C5-C4-N3	-3.75	121.55	126.72
3	B	2201	TG8	O4'-C1'-N9	3.49	114.80	108.09
3	B	2201	TG8	C4-C5-N7	-3.20	106.92	110.58
3	B	2202	TG8	C4-C5-N7	-3.16	106.97	110.58
3	B	2202	TG8	O1B-PB-O1A	2.87	114.26	104.64
3	B	2201	TG8	O1B-PB-O1A	2.82	114.09	104.64
3	B	2201	TG8	O3B-PB-O1A	2.81	114.04	104.64
3	B	2201	TG8	N3-C4-N9	2.80	131.94	127.17
3	B	2202	TG8	O3B-PB-O1A	2.76	113.89	104.64
3	B	2202	TG8	N3-C4-N9	2.71	131.78	127.17
3	B	2202	TG8	C4'-O4'-C1'	-2.64	103.64	109.47
3	B	2201	TG8	C2-N3-C4	2.64	118.27	111.83
3	B	2202	TG8	C2-N3-C4	2.61	118.20	111.83
3	B	2201	TG8	O3A-PA-O2A	-2.49	100.89	112.44
3	B	2201	TG8	C6-C5-C4	2.42	120.48	117.18
3	B	2202	TG8	O3A-PA-O2A	-2.41	101.24	112.44
3	B	2202	TG8	C6-C5-C4	2.37	120.42	117.18
3	B	2201	TG8	O3'-CA-OA	-2.02	120.26	123.55

There are no chirality outliers.

All (14) torsion outliers are listed below:

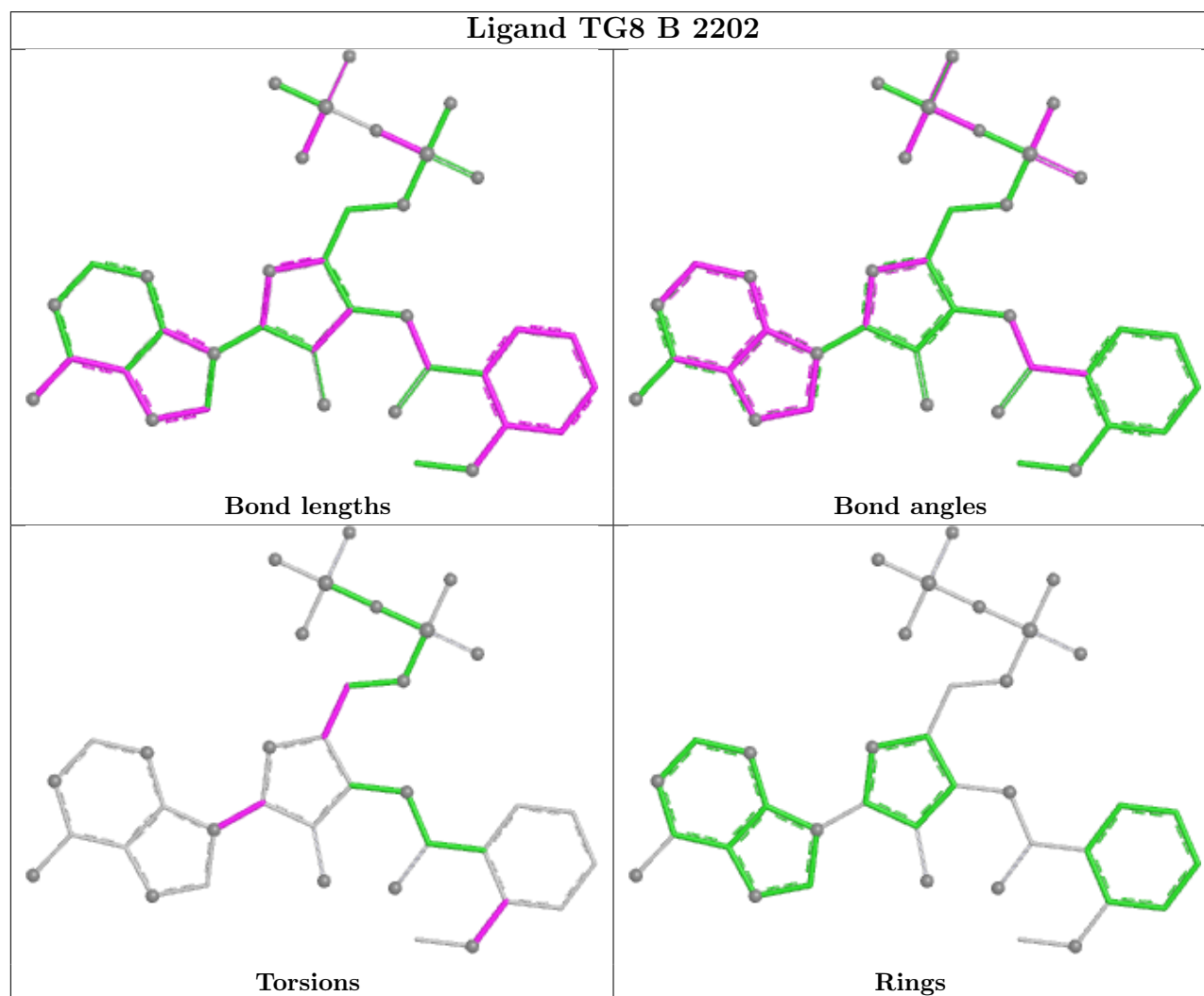
Mol	Chain	Res	Type	Atoms
3	B	2201	TG8	CA1-CA-O3'-C3'
3	B	2201	TG8	C5'-O5'-PA-O2A
3	B	2201	TG8	OA-CA-O3'-C3'
3	B	2202	TG8	O4'-C4'-C5'-O5'
3	B	2201	TG8	O3'-CA-CA1-CA6
3	B	2202	TG8	CA1-CA6-NA1-CA7
3	B	2202	TG8	CA5-CA6-NA1-CA7
3	B	2202	TG8	C2'-C1'-N9-C8
3	B	2201	TG8	C5'-O5'-PA-O1A
3	B	2201	TG8	CA1-CA6-NA1-CA7
3	B	2202	TG8	C2'-C1'-N9-C4
3	B	2201	TG8	O3'-CA-CA1-CA2
3	B	2201	TG8	OA-CA-CA1-CA6
3	B	2202	TG8	O4'-C1'-N9-C8

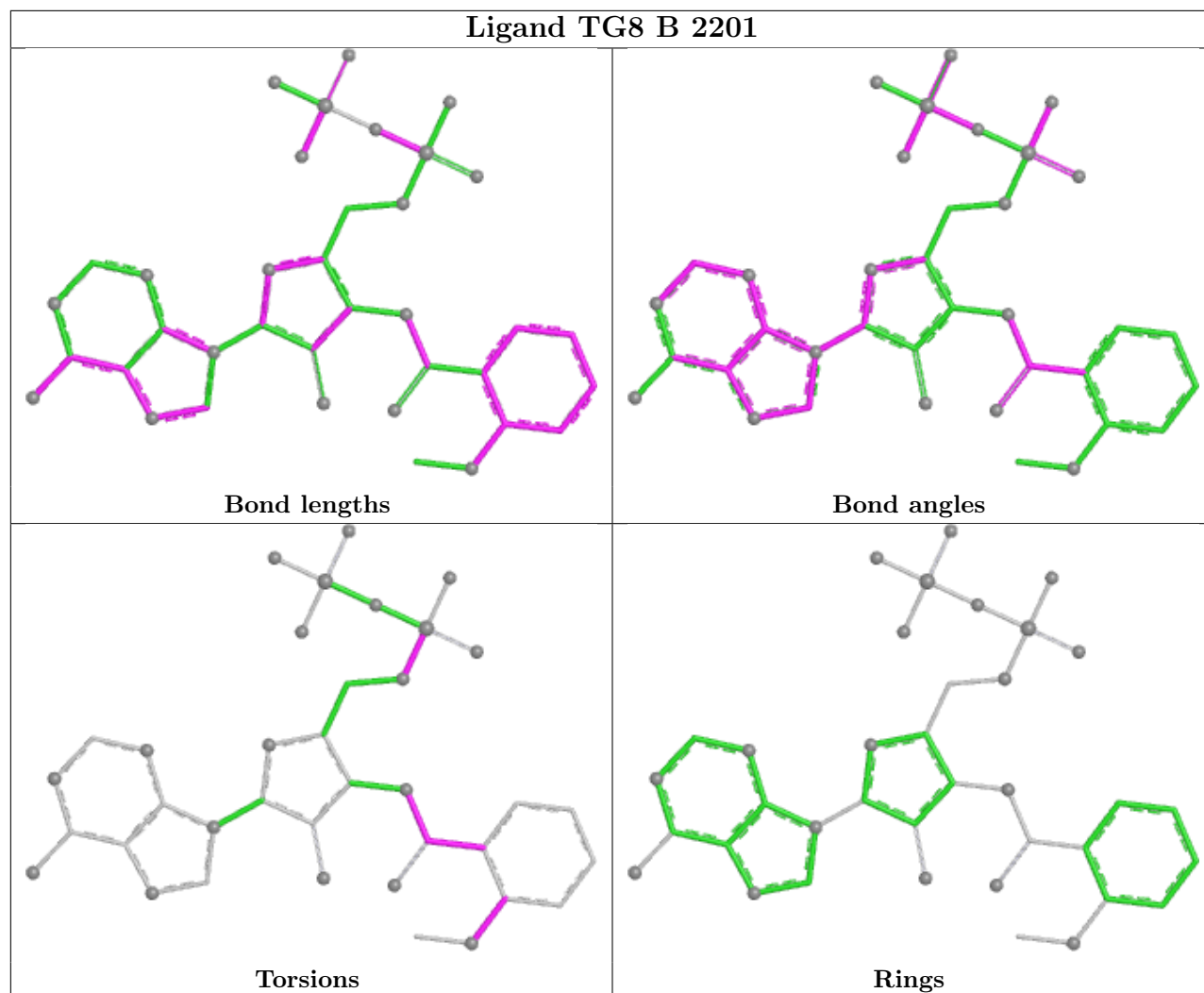
There are no ring outliers.

No monomer is involved in short contacts.

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	1725/1747 (98%)	0.30	88 (5%)	33 29	25, 55, 105, 131	0
2	J	262/263 (99%)	0.19	8 (3%)	51 48	30, 54, 96, 132	0
All	All	1987/2010 (98%)	0.29	96 (4%)	35 32	25, 54, 104, 132	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	2059	PRO	5.0
1	B	1968	SER	4.6
1	B	1889	VAL	4.4
1	B	1876	PRO	4.0
1	B	404	ALA	3.8
1	B	1601	LEU	3.8
1	B	403	LEU	3.8
1	B	1879	LEU	3.6
1	B	1761	TYR	3.5
2	J	2320	LEU	3.5
1	B	1997	LEU	3.5
1	B	572	ASP	3.5
1	B	575	LEU	3.4
1	B	859	PRO	3.3
1	B	529	GLY	3.3
1	B	2035	VAL	3.2
1	B	1860	ILE	3.2
1	B	1955	SER	3.1
1	B	1074	GLY	3.1
1	B	1858	ILE	3.0
1	B	2033	GLY	3.0
1	B	2027	ASP	3.0
1	B	1325	PHE	2.9
1	B	1168	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	2100	THR	2.8
2	J	2097	ILE	2.8
2	J	2061	GLY	2.7
1	B	2112	ALA	2.7
1	B	2047	VAL	2.7
1	B	1525	LEU	2.7
1	B	1859	PRO	2.6
1	B	1321	TYR	2.6
1	B	2069	GLY	2.6
1	B	527	MET	2.6
1	B	531	ILE	2.6
2	J	2060	LEU	2.6
1	B	1887	PRO	2.6
1	B	1604	LEU	2.6
1	B	2124	VAL	2.6
1	B	1994	ASN	2.6
1	B	525	ILE	2.5
1	B	1893	LEU	2.5
1	B	1904	LEU	2.5
1	B	1877	HIS	2.5
1	B	1832	PHE	2.5
1	B	1849	ILE	2.5
1	B	2004	ILE	2.5
1	B	1996	LEU	2.5
1	B	780	TYR	2.5
2	J	2063	MET	2.5
1	B	601	GLY	2.4
1	B	1964	PRO	2.4
1	B	1978	GLY	2.4
1	B	1995	ALA	2.4
1	B	1867	LEU	2.4
1	B	940	HIS	2.4
1	B	1261	PRO	2.4
1	B	1912	THR	2.4
1	B	1911	ASP	2.4
1	B	1910	SER	2.3
1	B	2034	PRO	2.3
1	B	698	ILE	2.3
1	B	1896	GLN	2.3
1	B	1908	LEU	2.3
1	B	571	GLY	2.3
1	B	1906	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1988	MET	2.3
1	B	1998	GLN	2.3
1	B	2106	LEU	2.3
1	B	2037	VAL	2.2
1	B	1171	GLY	2.2
1	B	569	LEU	2.2
1	B	1895	LEU	2.2
1	B	2083	THR	2.2
1	B	1607	SER	2.2
1	B	1158	HIS	2.2
1	B	1885	ASN	2.1
1	B	1961	LYS	2.1
1	B	1307	LEU	2.1
1	B	1963	LEU	2.1
1	B	1413	SER	2.1
1	B	1979	VAL	2.1
2	J	2121	ARG	2.1
1	B	754	GLU	2.1
1	B	1913	GLU	2.1
1	B	1600	TYR	2.1
1	B	1875	VAL	2.1
1	B	530	THR	2.1
1	B	1322	GLN	2.1
1	B	1151	GLU	2.0
1	B	2071	ALA	2.0
1	B	2123	SER	2.0
1	B	2036	VAL	2.0
1	B	577	LYS	2.0
1	B	2073	SER	2.0
1	B	1915	ILE	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](#)

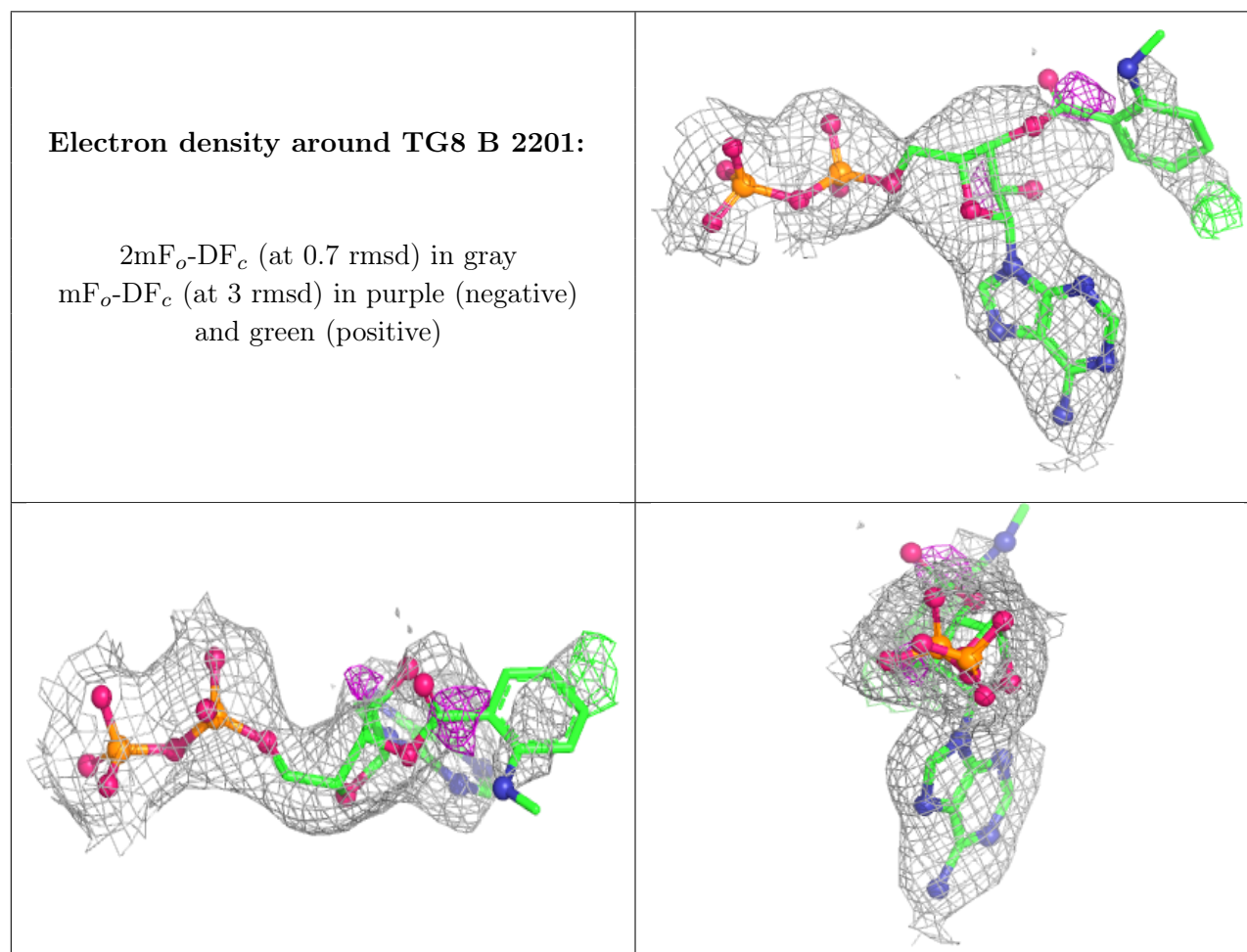
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

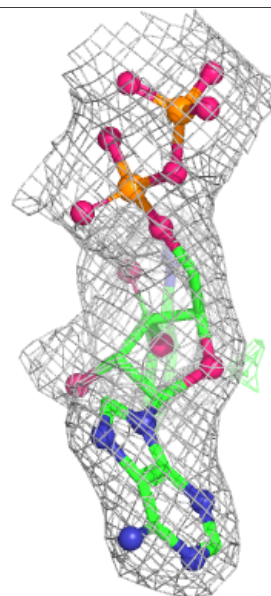
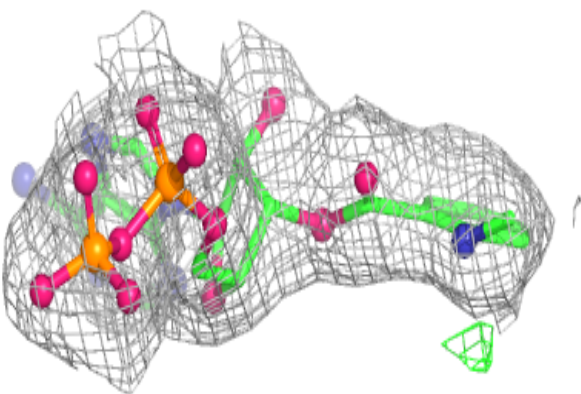
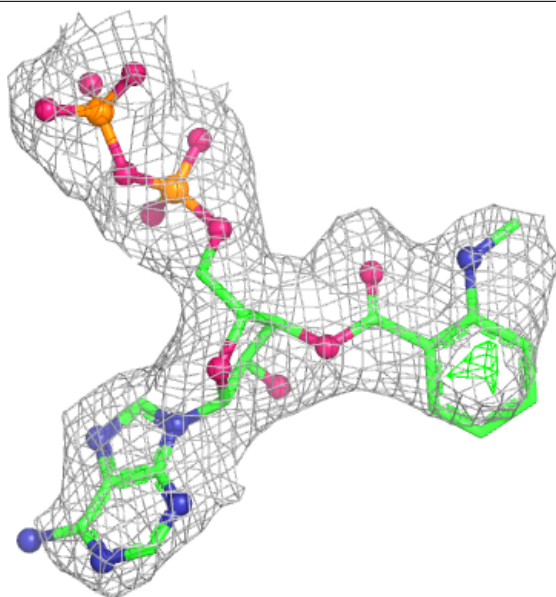
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TG8	B	2201	37/37	0.95	0.10	32,55,93,101	0
3	TG8	B	2202	37/37	0.95	0.09	36,55,70,76	0
4	MG	B	2203	1/1	0.99	0.06	34,34,34,34	0
4	MG	B	2204	1/1	1.00	0.04	38,38,38,38	0

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 TG8 B 2202:

$2mF_o-DF_c$ (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.