



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:43 AM UTC

PDB ID : 7BDI / pdb_00007bdi
Title : Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and ATPgammaS
Authors : Vester, K.; Santos, K.F.; Absmeier, E.; Wahl, M.C.
Deposited on : 2020-12-21
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

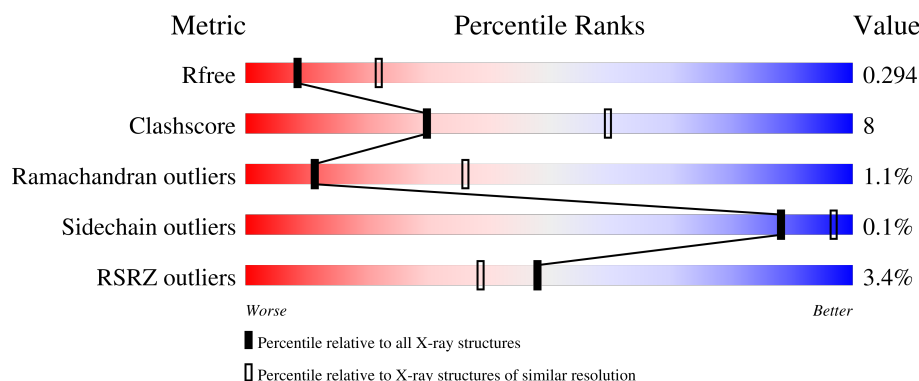
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

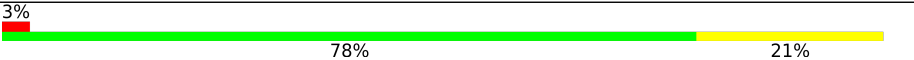
The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1747	
2	J	263	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16269 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

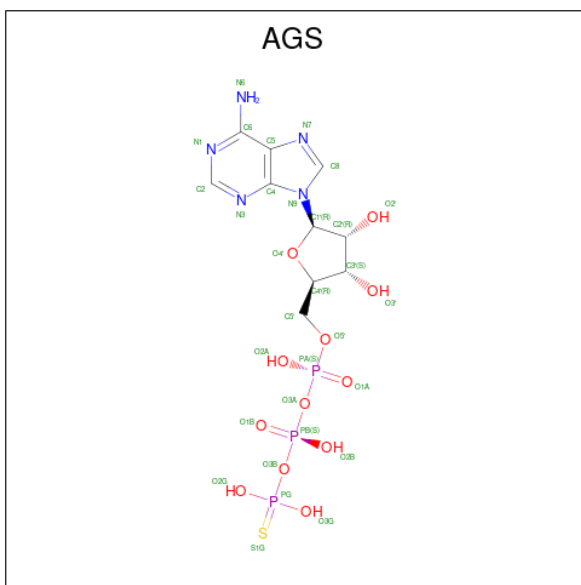
- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

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 PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
3	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	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

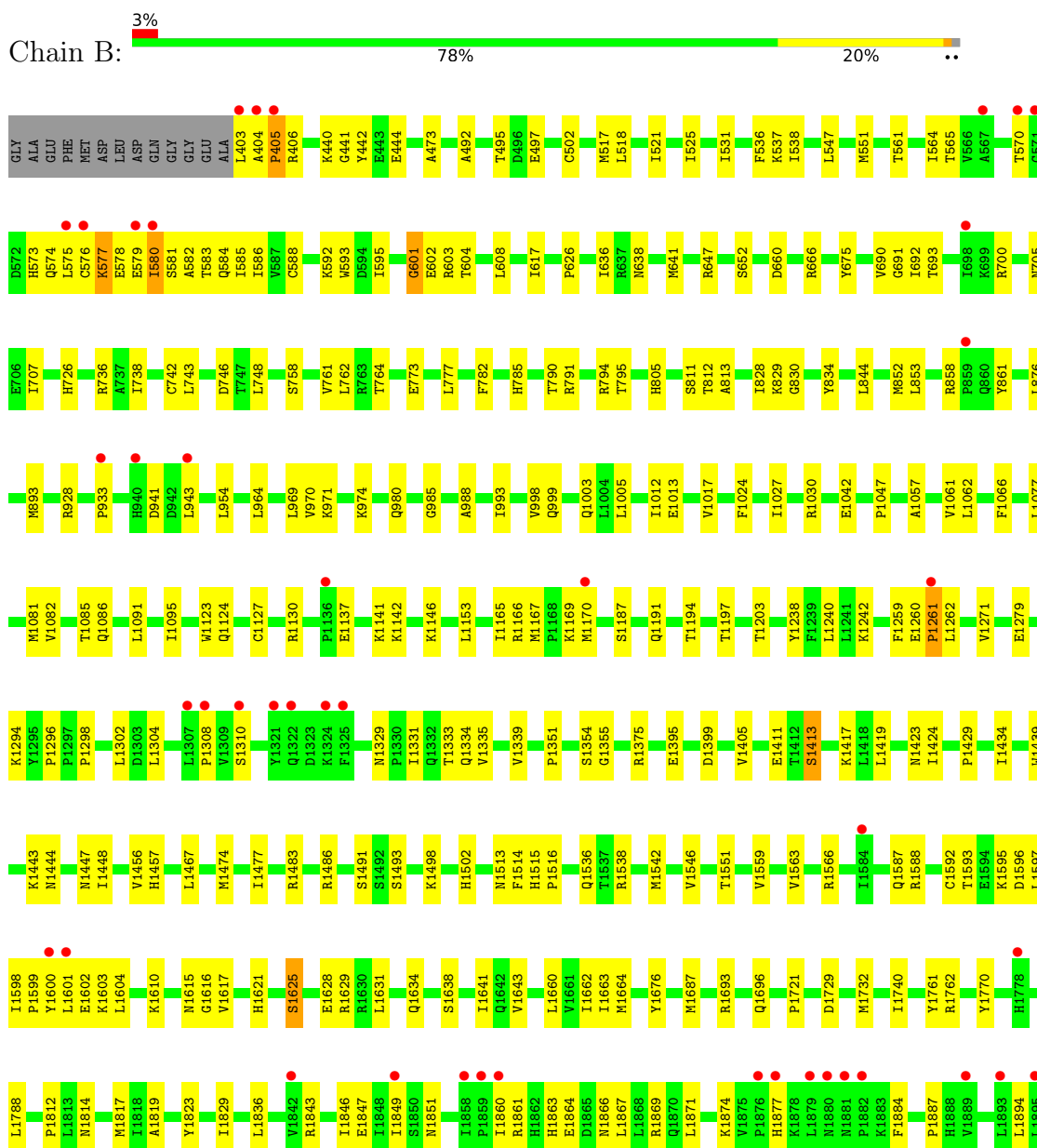
- Molecule 5 is water.

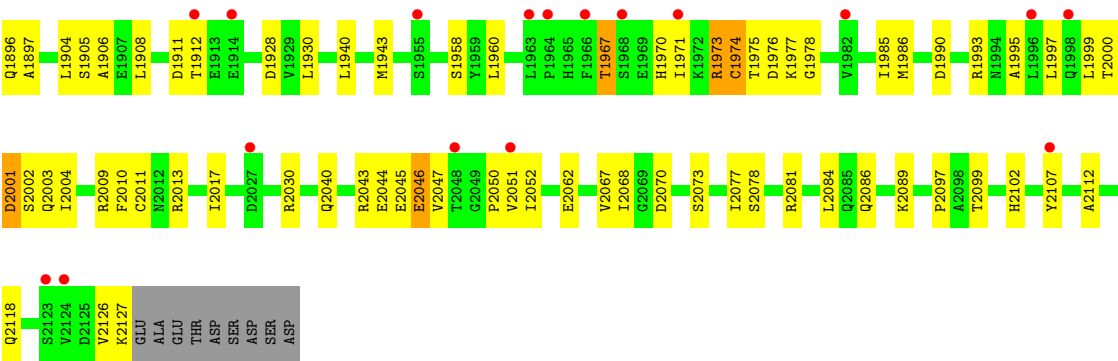
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	193	Total O 193 193	0	0
5	J	24	Total O 24 24	0	0

3 Residue-property plots

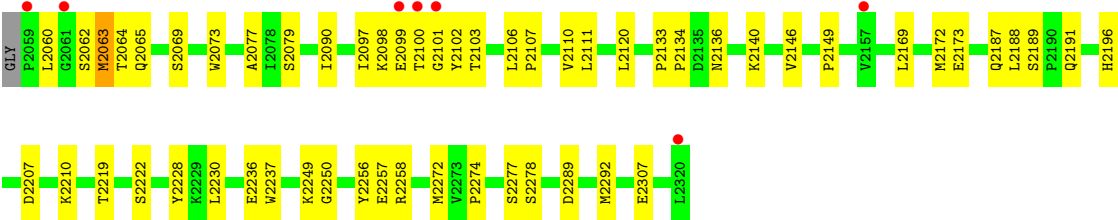
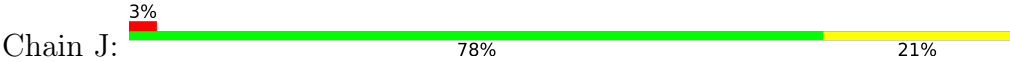
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	99.73Å 118.65Å 187.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.31 – 2.80 48.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.31-2.80) 99.8 (48.31-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.237 , 0.297 0.235 , 0.294	Depositor DCC
R_{free} test set	2101 reflections (3.78%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 22.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16269	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, 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	0.11	0/14164	0.30	0/19191
2	J	0.14	0/2185	0.35	0/2975
All	All	0.11	0/16349	0.31	0/22166

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
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1625	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	13870	0	14018	240	1
2	J	2118	0	2061	35	1
3	B	62	0	24	2	0
4	B	2	0	0	0	0
5	B	193	0	0	5	0
5	J	24	0	0	0	0
All	All	16269	0	16103	273	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 8.

All (273) 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:1602:GLU:C	1:B:1603:LYS:HE2	1.92	0.95
1:B:1604:LEU:HD12	1:B:1628:GLU:HG2	1.57	0.86
1:B:1958:SER:HB2	1:B:1971:ILE:HD13	1.59	0.84
1:B:579:GLU:HB2	1:B:580:ILE:HD12	1.65	0.78
1:B:1843:ARG:HH22	1:B:1847:GLU:HB2	1.51	0.74
1:B:1974:CYS:SG	1:B:1975:THR:N	2.62	0.72
1:B:971:LYS:HB2	1:B:980:GLN:HB3	1.72	0.72
1:B:1843:ARG:NH2	1:B:1847:GLU:HB2	2.07	0.69
1:B:2067:VAL:HB	1:B:2107:TYR:HB2	1.75	0.69
1:B:576:CYS:SG	1:B:1242:LYS:HE3	2.33	0.69
1:B:603:ARG:NH1	1:B:1676:TYR:OH	2.26	0.69
1:B:1973:ARG:HG2	1:B:1977:LYS:HE2	1.75	0.68
1:B:404:ALA:HB1	1:B:405:PRO:HD2	1.74	0.68
1:B:1843:ARG:HH21	1:B:1846:ILE:HG23	1.58	0.68
1:B:2000:THR:O	1:B:2002:SER:N	2.26	0.67
1:B:1732:MET:HE3	1:B:1788:LEU:HD21	1.75	0.67
1:B:547:LEU:HG	1:B:551:MET:HE2	1.77	0.67
1:B:1974:CYS:O	1:B:1978:GLY:N	2.28	0.67
1:B:525:ILE:HG22	1:B:531:ILE:HG13	1.76	0.66
2:J:2249:LYS:HE3	2:J:2249:LYS:HA	1.79	0.65
1:B:1603:LYS:HE2	1:B:1603:LYS:N	2.12	0.65
1:B:1434:ILE:HD13	1:B:1823:TYR:HB2	1.79	0.64
1:B:1904:LEU:HD11	1:B:1908:LEU:HB3	1.79	0.64
1:B:2045:GLU:CD	1:B:2046:GLU:H	2.06	0.63
1:B:1908:LEU:HA	1:B:1911:ASP:HB2	1.79	0.63
1:B:1985:ILE:O	1:B:1993:ARG:NH1	2.27	0.63
1:B:1960:LEU:HD23	1:B:1985:ILE:HD11	1.80	0.63
1:B:403:LEU:HA	1:B:954:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ILE:O	1:B:582:ALA:N	2.32	0.63
1:B:565:THR:HB	1:B:583:THR:HA	1.81	0.62
1:B:638:ASN:HA	1:B:641:MET:HE3	1.80	0.62
1:B:1308:PRO:HG2	1:B:1310:SER:HB3	1.81	0.62
1:B:691:GLY:HA3	1:B:876:LEU:HD11	1.82	0.62
1:B:1302:LEU:N	1:B:1334:GLN:OE1	2.33	0.62
2:J:2237:TRP:NE1	2:J:2249:LYS:O	2.28	0.62
1:B:1559:VAL:HG22	1:B:1660:LEU:HB3	1.82	0.62
1:B:1456:VAL:HG12	1:B:1491:SER:HB2	1.83	0.61
1:B:2001:ASP:HA	1:B:2004:ILE:HG12	1.81	0.61
1:B:2017:ILE:HG23	1:B:2043:ARG:HA	1.82	0.61
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.81	0.61
2:J:2090:ILE:HG21	2:J:2111:LEU:HD21	1.83	0.61
1:B:2030:ARG:HH22	1:B:2127:LYS:HD2	1.65	0.61
1:B:969:LEU:HD23	1:B:985:GLY:HA2	1.83	0.60
2:J:2103:THR:O	2:J:2140:LYS:N	2.34	0.60
1:B:785:HIS:HB3	1:B:811:SER:HB2	1.82	0.60
1:B:603:ARG:NH2	5:B:2302:HOH:O	2.27	0.60
1:B:1271:VAL:HG22	1:B:1279:GLU:HG3	1.84	0.60
1:B:582:ALA:O	1:B:584:GLN:NE2	2.35	0.59
1:B:1187:SER:HB3	1:B:1203:THR:HB	1.84	0.59
1:B:1625:SER:HB2	1:B:1628:GLU:H	1.67	0.59
1:B:743:LEU:HD12	1:B:748:LEU:HD11	1.85	0.59
1:B:2017:ILE:HD13	1:B:2084:LEU:HD23	1.85	0.59
1:B:580:ILE:HG12	1:B:586:ILE:HD11	1.84	0.58
2:J:2289:ASP:H	2:J:2292:MET:HE3	1.68	0.58
1:B:495:THR:HG22	1:B:497:GLU:H	1.69	0.58
1:B:1943:MET:HE1	1:B:2067:VAL:HG21	1.87	0.56
1:B:761:VAL:HA	1:B:764:THR:HG22	1.87	0.56
1:B:1169:LYS:HG2	1:B:1170:MET:HG3	1.86	0.56
1:B:577:LYS:C	1:B:579:GLU:H	2.13	0.56
1:B:1602:GLU:CA	1:B:1603:LYS:HE2	2.35	0.56
1:B:626:PRO:HG3	1:B:893:MET:HA	1.87	0.56
1:B:1419:LEU:HD22	1:B:1444:ASN:HB3	1.88	0.56
1:B:1617:VAL:HG22	1:B:1643:VAL:HB	1.87	0.56
2:J:2277:SER:OG	2:J:2278:SER:N	2.39	0.55
1:B:705:ASN:ND2	5:B:2316:HOH:O	2.39	0.55
1:B:1634:GLN:O	1:B:1638:SER:OG	2.21	0.55
1:B:858:ARG:HE	1:B:861:TYR:HB2	1.71	0.55
1:B:1990:ASP:HA	1:B:1993:ARG:HG2	1.88	0.55
1:B:492:ALA:HA	1:B:647:ARG:HH22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2106:LEU:HD12	2:J:2107:PRO:HD2	1.89	0.55
1:B:1294:LYS:NZ	5:B:2318:HOH:O	2.40	0.54
1:B:1967:THR:HG23	1:B:1970:HIS:ND1	2.22	0.54
1:B:933:PRO:HG3	1:B:943:LEU:HD22	1.90	0.54
1:B:577:LYS:HB2	1:B:579:GLU:HG3	1.90	0.54
1:B:1861:ARG:HB3	1:B:1863:HIS:CD2	2.42	0.54
1:B:2099:THR:HA	1:B:2126:VAL:HG13	1.90	0.53
2:J:2274:PRO:HB2	2:J:2277:SER:HB3	1.90	0.53
1:B:999:GLN:NE2	1:B:1003:GLN:OE1	2.40	0.53
1:B:521:ILE:HD13	1:B:564:ILE:HD13	1.90	0.53
1:B:1012:ILE:HG12	1:B:1047:PRO:HD2	1.91	0.53
1:B:1411:GLU:HG3	1:B:1413:SER:H	1.73	0.53
1:B:1877:HIS:HB2	1:B:1896:GLN:NE2	2.24	0.53
1:B:1999:LEU:HB3	1:B:2003:GLN:HB2	1.89	0.53
2:J:2140:LYS:NZ	2:J:2173:GLU:OE2	2.40	0.53
2:J:2189:SER:OG	2:J:2191:GLN:OE1	2.27	0.53
1:B:406:ARG:HD3	1:B:954:LEU:HG	1.91	0.52
1:B:1153:LEU:HD12	1:B:1153:LEU:H	1.73	0.52
1:B:636:ILE:HD13	1:B:666:ARG:HG3	1.91	0.52
1:B:1062:LEU:HB3	1:B:1081:MET:HG3	1.92	0.52
1:B:2040:GLN:HG3	1:B:2089:LYS:HG2	1.91	0.52
1:B:602:GLU:HA	1:B:604:THR:HG22	1.92	0.52
1:B:1597:LEU:O	1:B:1601:LEU:N	2.43	0.52
1:B:1013:GLU:O	1:B:1017:VAL:HG23	2.10	0.52
1:B:1298:PRO:HB3	1:B:1515:HIS:CG	2.45	0.52
1:B:758:SER:HB3	1:B:805:HIS:CD2	2.45	0.51
1:B:1082:VAL:O	1:B:1086:GLN:HG2	2.10	0.51
1:B:1819:ALA:HB2	1:B:1829:ILE:HG13	1.91	0.51
1:B:758:SER:HB3	1:B:805:HIS:HD2	1.75	0.51
1:B:444:GLU:HG2	1:B:690:VAL:HG22	1.93	0.51
1:B:617:ILE:HG22	1:B:652:SER:HB2	1.91	0.51
1:B:1551:THR:HG22	1:B:1588:ARG:HH12	1.76	0.51
1:B:1604:LEU:HD12	1:B:1628:GLU:CG	2.36	0.51
1:B:537:LYS:HE2	1:B:608:LEU:HD13	1.92	0.51
1:B:2043:ARG:NH2	1:B:2062:GLU:OE2	2.27	0.51
1:B:1355:GLY:HA2	3:B:2202:AGS:O2A	2.10	0.50
1:B:660:ASP:OD2	1:B:928:ARG:NH1	2.44	0.50
1:B:1986:MET:HE2	1:B:2011:CYS:HB3	1.93	0.50
1:B:576:CYS:O	1:B:578:GLU:N	2.42	0.50
1:B:1600:TYR:HB3	1:B:1631:LEU:HD21	1.92	0.50
1:B:1335:VAL:O	1:B:1339:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:LYS:HD3	1:B:580:ILE:HG21	1.93	0.50
1:B:726:HIS:NE2	1:B:830:GLY:O	2.39	0.50
1:B:1296:PRO:HG2	1:B:1498:LYS:CE	2.42	0.50
1:B:1693:ARG:HB3	1:B:1696:GLN:HB2	1.92	0.50
1:B:601:GLY:H	1:B:1536:GLN:HG2	1.76	0.50
1:B:1439:TRP:CD2	1:B:1477:ILE:HG12	2.47	0.50
1:B:2013:ARG:HD3	1:B:2052:ILE:HD11	1.93	0.50
1:B:1057:ALA:O	1:B:1061:VAL:HG23	2.12	0.49
1:B:1296:PRO:HG2	1:B:1498:LYS:HE3	1.94	0.49
1:B:1940:LEU:HA	1:B:1943:MET:HE3	1.95	0.49
1:B:1024:PHE:HB3	1:B:1027:ILE:HD12	1.94	0.49
1:B:1260:GLU:O	1:B:1262:LEU:N	2.45	0.49
1:B:993:ILE:HD12	1:B:1091:LEU:HD23	1.93	0.49
1:B:2046:GLU:HA	1:B:2086:GLN:OE1	2.12	0.49
1:B:1729:ASP:OD1	1:B:1729:ASP:N	2.46	0.49
1:B:1846:ILE:HA	1:B:1849:ILE:HG22	1.95	0.49
1:B:1864:GLU:HG3	1:B:1867:LEU:HB3	1.95	0.48
1:B:1142:LYS:O	1:B:1146:LYS:HG2	2.13	0.48
1:B:1165:ILE:HD12	1:B:1167:MET:HE3	1.96	0.48
1:B:1194:THR:HB	1:B:1197:THR:H	1.78	0.48
1:B:812:THR:OG1	1:B:813:ALA:N	2.45	0.48
1:B:1866:ASN:HA	1:B:1869:ARG:HB2	1.95	0.48
1:B:1339:VAL:HA	1:B:1486:ARG:HH22	1.78	0.48
1:B:1515:HIS:NE2	1:B:1721:PRO:HG3	2.28	0.48
1:B:1444:ASN:HA	1:B:1447:ASN:HD21	1.77	0.48
1:B:964:LEU:HB3	1:B:970:VAL:HG23	1.94	0.48
1:B:1592:CYS:SG	1:B:1596:ASP:HB2	2.54	0.48
1:B:2045:GLU:OE2	1:B:2047:VAL:HB	2.14	0.48
1:B:570:THR:HB	1:B:573:HIS:CE1	2.50	0.47
1:B:834:TYR:OH	1:B:1030:ARG:NH1	2.46	0.47
1:B:1405:VAL:HG12	1:B:1424:ILE:HB	1.96	0.47
1:B:1395:GLU:HA	1:B:1399:ASP:HB2	1.96	0.47
1:B:1836:LEU:HD22	1:B:1930:LEU:HD21	1.96	0.47
1:B:441:GLY:O	1:B:693:THR:OG1	2.31	0.47
1:B:692:ILE:HG21	1:B:700:ARG:HG3	1.97	0.47
1:B:2068:ILE:HG22	1:B:2077:ILE:HB	1.97	0.47
1:B:1498:LYS:HB2	1:B:1498:LYS:HE2	1.70	0.46
1:B:1904:LEU:CD1	1:B:1908:LEU:HB3	2.44	0.46
1:B:1616:GLY:HA2	1:B:1641:ILE:HG22	1.97	0.46
1:B:1894:LEU:HG	1:B:1912:THR:HG23	1.98	0.46
1:B:1592:CYS:SG	1:B:1593:THR:N	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1625:SER:HB2	1:B:1628:GLU:N	2.31	0.46
2:J:2146:VAL:HG22	2:J:2272:MET:HB2	1.98	0.46
2:J:2219:THR:OG1	2:J:2222:SER:OG	2.24	0.46
1:B:1814:ASN:HA	1:B:1817:MET:HE2	1.98	0.46
1:B:988:ALA:HB2	1:B:998:VAL:HG11	1.96	0.46
1:B:1871:LEU:HD21	1:B:1897:ALA:HB2	1.97	0.46
2:J:2073:TRP:O	2:J:2077:ALA:N	2.47	0.46
1:B:502:CYS:HB2	1:B:675:TYR:HA	1.98	0.46
1:B:1375:ARG:HH22	1:B:1447:ASN:HD21	1.64	0.46
1:B:1958:SER:CB	1:B:1971:ILE:HD13	2.37	0.46
2:J:2099:GLU:OE1	2:J:2101:GLY:N	2.44	0.46
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.51	0.45
1:B:2009:ARG:HE	1:B:2013:ARG:NH2	2.14	0.45
2:J:2079:SER:HB3	2:J:2120:LEU:HD12	1.98	0.45
1:B:1127:CYS:O	1:B:1130:ARG:HG2	2.16	0.45
1:B:1137:GLU:C	1:B:1141:LYS:HZ1	2.24	0.45
1:B:1329:ASN:O	1:B:1333:THR:HG23	2.17	0.45
1:B:1566:ARG:HG3	1:B:1621:HIS:CG	2.51	0.45
1:B:690:VAL:HG11	1:B:707:ILE:HD13	1.98	0.45
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	1.99	0.45
1:B:2000:THR:O	1:B:2000:THR:HG22	2.16	0.45
1:B:517:MET:HG2	1:B:538:ILE:HG21	1.98	0.45
1:B:517:MET:HE3	1:B:585:ILE:HD13	1.98	0.45
1:B:1502:HIS:CE1	1:B:1762:ARG:HE	2.35	0.45
1:B:2102:HIS:HD2	1:B:2126:VAL:HG11	1.81	0.45
2:J:2188:LEU:HD12	2:J:2228:TYR:CD2	2.52	0.45
1:B:736:ARG:NH2	1:B:773:GLU:OE2	2.50	0.45
1:B:1296:PRO:HD2	1:B:1498:LYS:NZ	2.32	0.45
1:B:1625:SER:HB2	1:B:1628:GLU:HG3	1.99	0.45
1:B:1871:LEU:HD12	1:B:1874:LYS:HB2	1.99	0.45
1:B:742:CYS:O	1:B:746:ASP:N	2.50	0.45
1:B:1601:LEU:HD11	1:B:1610:LYS:HB3	1.99	0.44
1:B:1598:ILE:HD12	1:B:1599:PRO:HD3	1.98	0.44
1:B:588:CYS:SG	1:B:593:TRP:HB2	2.57	0.44
1:B:1587:GLN:HG2	1:B:1615:ASN:HA	1.98	0.44
1:B:1976:ASP:OD2	1:B:1976:ASP:N	2.50	0.44
2:J:2060:LEU:HD12	2:J:2063:MET:HA	2.00	0.44
1:B:518:LEU:HD23	1:B:518:LEU:HA	1.89	0.44
1:B:1995:ALA:O	1:B:1997:LEU:N	2.49	0.44
1:B:2013:ARG:HG2	1:B:2047:VAL:HG23	2.00	0.44
2:J:2196:HIS:HD2	2:J:2230:LEU:HD22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1166:ARG:HA	1:B:1166:ARG:HH11	1.83	0.43
1:B:1448:ILE:HD11	1:B:1474:MET:HE2	2.00	0.43
1:B:1546:VAL:HG22	1:B:1662:ILE:HG21	2.00	0.43
1:B:1871:LEU:HA	1:B:1874:LYS:HB2	1.99	0.43
1:B:1042:GLU:HB2	2:J:2069:SER:O	2.18	0.43
1:B:1429:PRO:HG3	1:B:1467:LEU:HD13	2.00	0.43
3:B:2202:AGS:H8	3:B:2202:AGS:H2'	1.60	0.43
2:J:2099:GLU:CD	2:J:2100:THR:H	2.26	0.43
2:J:2107:PRO:HG2	2:J:2110:VAL:HG22	1.99	0.43
1:B:790:THR:O	1:B:794:ARG:HG3	2.18	0.43
1:B:1538:ARG:HG2	1:B:1542:MET:HE3	2.01	0.43
1:B:1302:LEU:HB2	1:B:1304:LEU:HG	2.00	0.43
1:B:974:LYS:H	1:B:974:LYS:HD2	1.84	0.43
2:J:2064:THR:OG1	2:J:2065:GLN:N	2.52	0.43
1:B:828:ILE:HD13	1:B:852:MET:HE3	2.01	0.42
2:J:2237:TRP:CD1	2:J:2250:GLY:HA3	2.53	0.42
1:B:521:ILE:HG12	1:B:536:PHE:CZ	2.54	0.42
1:B:2043:ARG:NH1	1:B:2084:LEU:O	2.33	0.42
1:B:2045:GLU:CG	1:B:2046:GLU:H	2.31	0.42
1:B:1123:TRP:HB3	2:J:2307:GLU:OE2	2.19	0.42
1:B:1170:MET:HE3	1:B:1170:MET:HB2	1.87	0.42
1:B:1191:GLN:HB3	1:B:1770:TYR:CD2	2.54	0.42
1:B:1262:LEU:HD23	1:B:1262:LEU:HA	1.76	0.42
1:B:2068:ILE:HB	1:B:2078:SER:HB2	2.00	0.42
2:J:2169:LEU:HA	2:J:2172:MET:HE3	2.02	0.42
1:B:473:ALA:HB1	1:B:561:THR:HG21	2.01	0.42
1:B:592:LYS:O	1:B:595:ILE:HG22	2.20	0.42
1:B:829:LYS:NZ	5:B:2316:HOH:O	2.52	0.42
1:B:1259:PHE:HD2	1:B:1261:PRO:HG2	1.83	0.42
1:B:1417:LYS:N	1:B:1417:LYS:HD2	2.35	0.42
1:B:1905:SER:OG	1:B:1906:ALA:N	2.53	0.42
2:J:2100:THR:HG21	2:J:2257:GLU:HG3	2.01	0.42
1:B:844:LEU:HD23	1:B:844:LEU:HA	1.89	0.42
1:B:1423:ASN:O	1:B:1424:ILE:HD13	2.19	0.42
1:B:573:HIS:CG	1:B:573:HIS:O	2.73	0.42
1:B:576:CYS:SG	1:B:1240:LEU:HD21	2.60	0.42
1:B:1457:HIS:HB3	1:B:1491:SER:OG	2.19	0.42
1:B:1663:ILE:HD13	1:B:1687:MET:HE3	2.02	0.42
1:B:1869:ARG:HG2	1:B:1884:PHE:CE1	2.55	0.42
2:J:2097:ILE:HG21	2:J:2258:ARG:NE	2.35	0.42
1:B:521:ILE:HG12	1:B:536:PHE:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:853:LEU:HD23	1:B:853:LEU:HA	1.93	0.41
1:B:1417:LYS:HD2	1:B:1417:LYS:H	1.84	0.41
1:B:1905:SER:HB3	1:B:1908:LEU:HB2	2.02	0.41
1:B:577:LYS:C	1:B:579:GLU:N	2.77	0.41
1:B:791:ARG:HE	1:B:795:THR:HG23	1.86	0.41
1:B:1595:LYS:O	1:B:1598:ILE:HG13	2.20	0.41
1:B:1740:ILE:HG22	1:B:1812:PRO:HB3	2.01	0.41
2:J:2097:ILE:HG12	2:J:2258:ARG:NH1	2.36	0.41
1:B:1625:SER:O	1:B:1629:ARG:HG3	2.19	0.41
1:B:2051:VAL:HG11	1:B:2112:ALA:HB1	2.03	0.41
1:B:1005:LEU:HD11	1:B:1095:ILE:HG23	2.02	0.41
1:B:1443:LYS:H	1:B:1443:LYS:HG2	1.64	0.41
2:J:2207:ASP:HB3	2:J:2210:LYS:HB2	2.02	0.41
1:B:1860:ILE:HD11	1:B:1887:PRO:CD	2.50	0.41
1:B:1563:VAL:HG12	1:B:1664:MET:HE2	2.02	0.41
1:B:2017:ILE:O	1:B:2118:GLN:NE2	2.54	0.41
2:J:2133:PRO:HG2	2:J:2136:ASN:HB2	2.03	0.41
2:J:2187:GLN:HB2	2:J:2256:TYR:OH	2.21	0.41
1:B:1124:GLN:N	2:J:2307:GLU:OE2	2.54	0.41
1:B:1493:SER:HB3	1:B:1514:PHE:O	2.20	0.41
1:B:2044:GLU:O	1:B:2044:GLU:HG2	2.21	0.41
2:J:2097:ILE:HG12	2:J:2258:ARG:HH11	1.85	0.41
1:B:442:TYR:HE1	1:B:444:GLU:HG3	1.86	0.41
1:B:1602:GLU:N	1:B:1603:LYS:HE2	2.36	0.41
1:B:2070:ASP:OD2	1:B:2073:SER:OG	2.25	0.41
1:B:575:LEU:HD12	1:B:576:CYS:HB2	2.03	0.41
1:B:2010:PHE:HA	1:B:2052:ILE:HD12	2.03	0.41
2:J:2149:PRO:HD3	2:J:2274:PRO:HG3	2.03	0.41
1:B:1847:GLU:OE2	1:B:1847:GLU:HA	2.20	0.40
1:B:1513:ASN:ND2	5:B:2306:HOH:O	2.30	0.40
1:B:574:GLN:N	1:B:574:GLN:OE1	2.55	0.40
1:B:575:LEU:HD22	1:B:1238:TYR:OH	2.22	0.40
1:B:762:LEU:HD23	1:B:762:LEU:HA	1.87	0.40
1:B:777:LEU:HB3	1:B:782:PHE:HB2	2.03	0.40
1:B:1077:LEU:HD23	1:B:1077:LEU:HA	1.96	0.40
1:B:1928:ASP:OD1	1:B:2081:ARG:NH2	2.54	0.40
1:B:1973:ARG:CG	1:B:1977:LYS:HE2	2.47	0.40
1:B:785:HIS:CE1	1:B:794:ARG:HD2	2.57	0.40
1:B:2000:THR:C	1:B:2002:SER:N	2.79	0.40
2:J:2098:LYS:HB2	2:J:2098:LYS:HE3	1.82	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1761:TYR:OH	2:J:2065:GLN:OE1[4_555]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1723/1747 (99%)	1622 (94%)	84 (5%)	17 (1%)	12	38
2	J	260/263 (99%)	231 (89%)	24 (9%)	5 (2%)	6	22
All	All	1983/2010 (99%)	1853 (93%)	108 (5%)	22 (1%)	11	36

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	405	PRO
1	B	581	SER
1	B	1973	ARG
1	B	440	LYS
1	B	580	ILE
1	B	1967	THR
1	B	2001	ASP
1	B	2046	GLU
1	B	2097	PRO
2	J	2063	MET
2	J	2236	GLU
1	B	577	LYS
2	J	2062	SER
2	J	2102	TYR
1	B	1483	ARG
1	B	1851	ASN
1	B	1974	CYS
1	B	2050	PRO

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Mol	Chain	Res	Type
2	J	2134	PRO
1	B	601	GLY
1	B	738	ILE
1	B	1261	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	1544/1560 (99%)	1542 (100%)	2 (0%)	88	97
2	J	236/236 (100%)	236 (100%)	0	100	100
All	All	1780/1796 (99%)	1778 (100%)	2 (0%)	88	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	941	ASP
1	B	1413	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	607	GLN
1	B	805	HIS
1	B	1002	ASN
1	B	1086	GLN
1	B	1101	ASN
1	B	1235	HIS
1	B	1337	ASN
1	B	1341	ASN
1	B	1531	ASN
1	B	1548	HIS
1	B	1553	HIS
1	B	1568	GLN

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Mol	Chain	Res	Type
1	B	1692	ASN
1	B	1851	ASN
1	B	1857	ASN
1	B	1862	HIS
1	B	1870	GLN
1	B	1877	HIS
1	B	1888	HIS
1	B	1962	GLN
1	B	2086	GLN
2	J	2089	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	AGS	B	2202	4	32,33,33	3.55	15 (46%)	45,52,52	1.96	12 (26%)
3	AGS	B	2201	4	32,33,33	3.53	15 (46%)	45,52,52	1.99	13 (28%)

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	AGS	B	2202	4	-	5/21/38/38	0/3/3/3
3	AGS	B	2201	4	-	6/21/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2202	AGS	C3'-C4'	-9.99	1.27	1.53
3	B	2201	AGS	C3'-C4'	-9.71	1.28	1.53
3	B	2201	AGS	C2'-C1'	-8.65	1.26	1.53
3	B	2202	AGS	C2'-C1'	-8.48	1.26	1.53
3	B	2202	AGS	O4'-C1'	6.71	1.57	1.42
3	B	2201	AGS	O4'-C1'	6.56	1.57	1.42
3	B	2202	AGS	PB-O3B	5.38	1.65	1.59
3	B	2201	AGS	PB-O3B	5.25	1.65	1.59
3	B	2201	AGS	C2'-C3'	5.03	1.67	1.53
3	B	2202	AGS	C2'-C3'	4.97	1.66	1.53
3	B	2201	AGS	O4'-C4'	4.55	1.55	1.45
3	B	2202	AGS	O4'-C4'	4.38	1.54	1.45
3	B	2201	AGS	C6-N6	4.35	1.45	1.34
3	B	2202	AGS	C6-N6	4.35	1.45	1.34
3	B	2202	AGS	PG-O2G	3.87	1.67	1.54
3	B	2201	AGS	PG-O2G	3.83	1.67	1.54
3	B	2201	AGS	PG-O3G	3.44	1.65	1.54
3	B	2202	AGS	PG-O3G	3.42	1.65	1.54
3	B	2202	AGS	PA-O3A	2.95	1.62	1.59
3	B	2201	AGS	C5-C4	-2.91	1.33	1.39
3	B	2202	AGS	C5-C4	-2.90	1.33	1.39
3	B	2201	AGS	PA-O3A	2.87	1.62	1.59
3	B	2202	AGS	C5-N7	-2.83	1.33	1.39
3	B	2202	AGS	O2'-C2'	2.83	1.50	1.43
3	B	2201	AGS	O2'-C2'	2.82	1.49	1.43
3	B	2201	AGS	C5-N7	-2.81	1.33	1.39
3	B	2201	AGS	C5'-C4'	2.74	1.59	1.51
3	B	2202	AGS	C5'-C4'	2.71	1.59	1.51
3	B	2201	AGS	C8-N9	-2.69	1.33	1.37
3	B	2202	AGS	C8-N9	-2.65	1.33	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2201	AGS	N3-C2-N1	-5.68	119.99	128.58
3	B	2202	AGS	N3-C2-N1	-5.65	120.02	128.58
3	B	2202	AGS	C5-C4-N3	-4.84	120.06	126.72
3	B	2201	AGS	C5-C4-N3	-4.82	120.08	126.72
3	B	2201	AGS	N9-C8-N7	-4.49	107.57	113.94
3	B	2202	AGS	N9-C8-N7	-4.42	107.66	113.94
3	B	2201	AGS	C1'-N9-C8	-3.38	119.59	127.09
3	B	2202	AGS	C1'-N9-C8	-3.37	119.62	127.09
3	B	2201	AGS	C2-N3-C4	3.34	119.98	111.83
3	B	2202	AGS	C2-N3-C4	3.33	119.96	111.83
3	B	2201	AGS	C5-N7-C8	3.02	108.20	103.45
3	B	2202	AGS	C5-N7-C8	2.97	108.12	103.45
3	B	2202	AGS	N3-C4-N9	2.96	132.19	127.17
3	B	2201	AGS	N3-C4-N9	2.93	132.16	127.17
3	B	2201	AGS	C4-N9-C8	2.60	108.47	105.74
3	B	2202	AGS	C3'-C2'-C1'	2.53	106.26	101.46
3	B	2202	AGS	PB-O3B-PG	-2.53	123.90	133.17
3	B	2202	AGS	C4-N9-C8	2.53	108.39	105.74
3	B	2201	AGS	PB-O3B-PG	-2.48	124.11	133.17
3	B	2202	AGS	C4-N9-C1'	2.29	131.98	126.63
3	B	2201	AGS	C4-N9-C1'	2.27	131.94	126.63
3	B	2201	AGS	C4'-O4'-C1'	-2.26	104.48	109.47
3	B	2201	AGS	C4-C5-N7	-2.25	108.01	110.58
3	B	2201	AGS	C2'-C3'-C4'	2.25	106.95	102.61
3	B	2202	AGS	C4-C5-N7	-2.19	108.08	110.58

There are no chirality outliers.

All (11) torsion outliers are listed below:

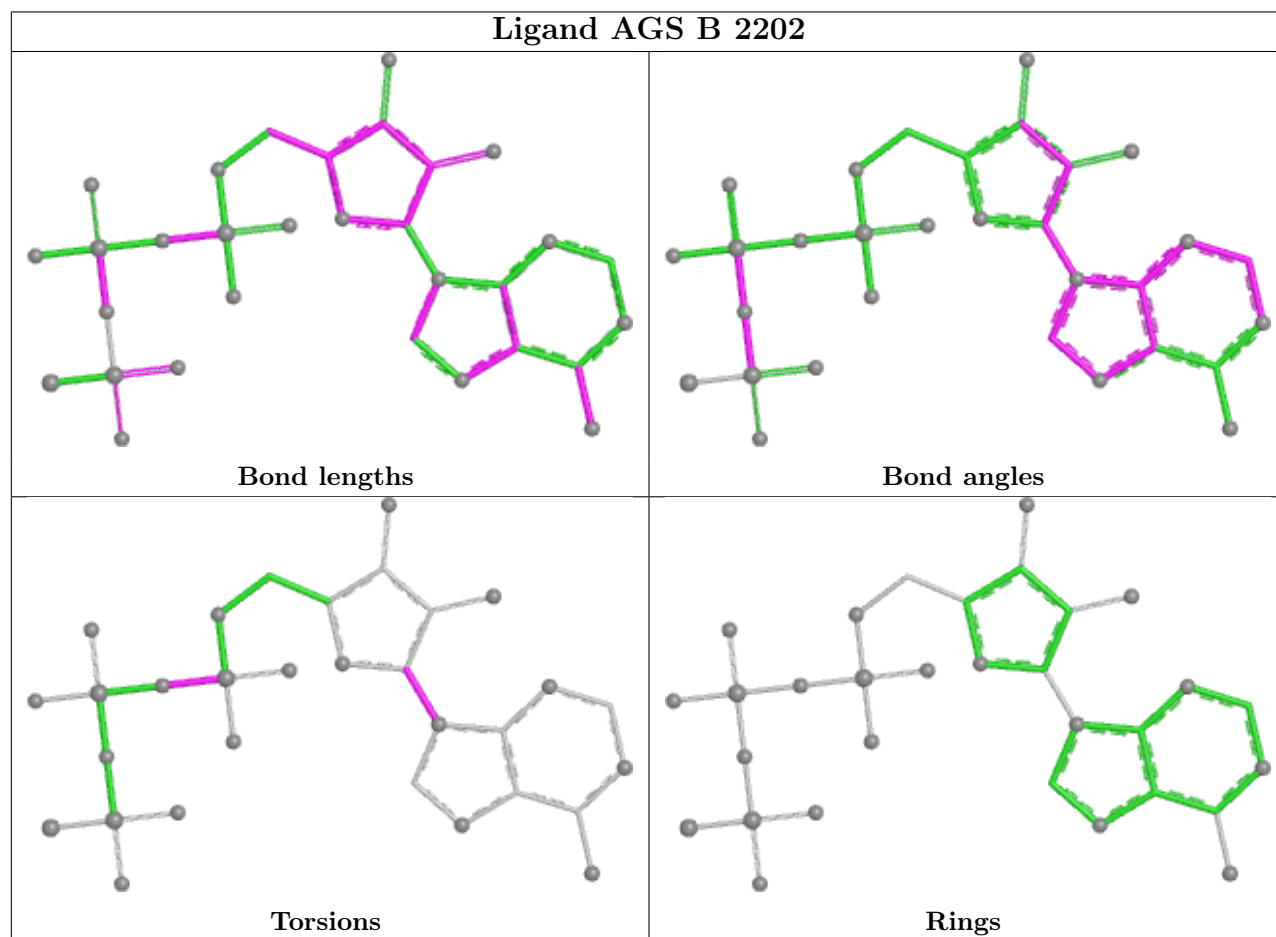
Mol	Chain	Res	Type	Atoms
3	B	2201	AGS	PB-O3B-PG-O2G
3	B	2201	AGS	PB-O3B-PG-O3G
3	B	2201	AGS	PA-O3A-PB-O1B
3	B	2201	AGS	PG-O3B-PB-O1B
3	B	2202	AGS	C2'-C1'-N9-C8
3	B	2202	AGS	PB-O3A-PA-O1A
3	B	2202	AGS	C2'-C1'-N9-C4
3	B	2201	AGS	C2'-C1'-N9-C8
3	B	2202	AGS	O4'-C1'-N9-C8
3	B	2201	AGS	PG-O3B-PB-O2B
3	B	2202	AGS	PB-O3A-PA-O2A

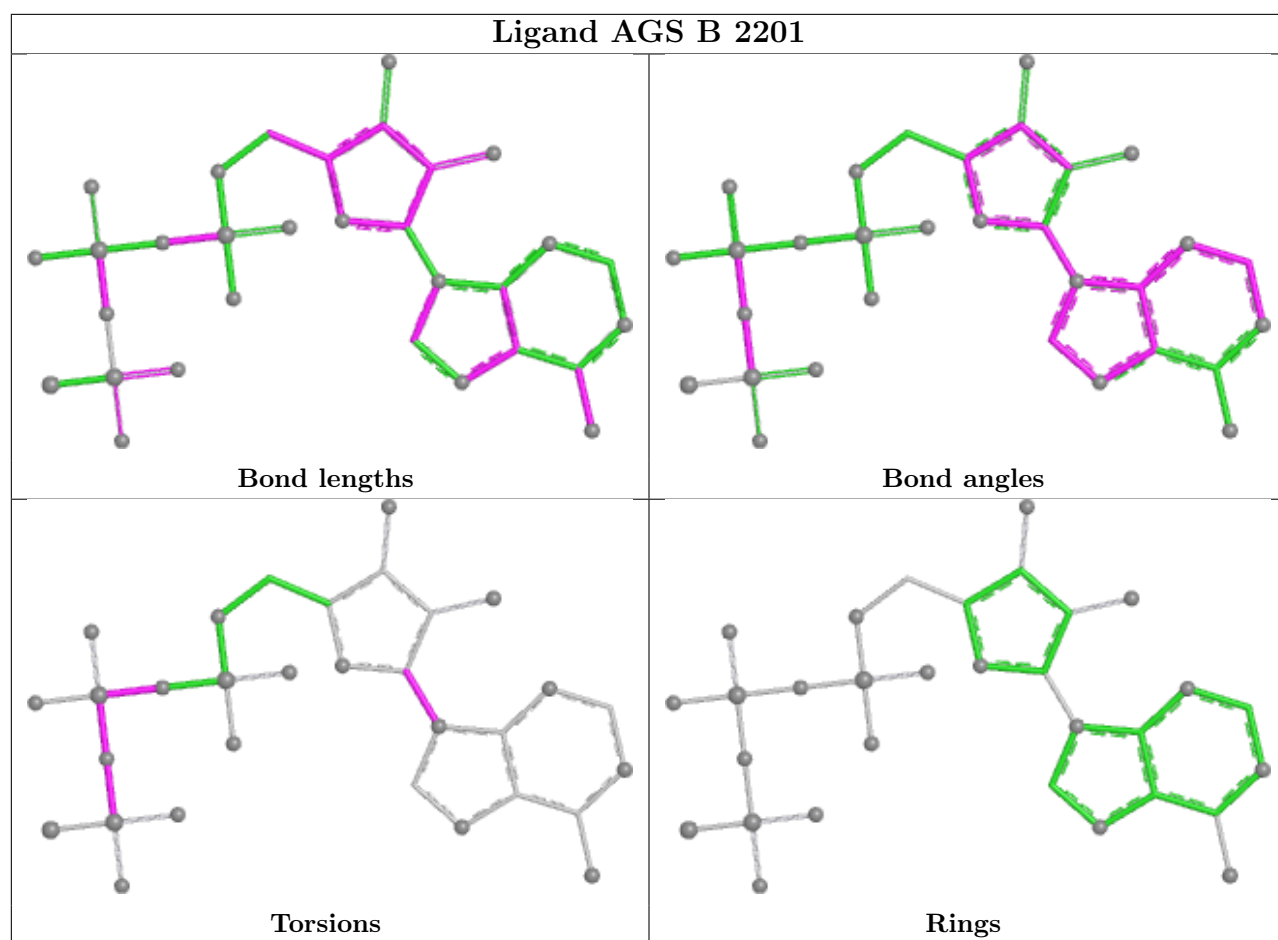
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2202	AGS	2	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	1725/1747 (98%)	0.18	60 (3%) 47 38	24, 52, 95, 124	0
2	J	262/263 (99%)	0.18	7 (2%) 56 46	29, 53, 83, 128	0
All	All	1987/2010 (98%)	0.18	67 (3%) 48 39	24, 52, 95, 128	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1889	VAL	4.0
1	B	1893	LEU	3.7
1	B	1881	ASN	3.6
1	B	1310	SER	3.6
1	B	2124	VAL	3.4
1	B	933	PRO	3.3
1	B	1601	LEU	3.2
1	B	580	ILE	3.1
1	B	1325	PHE	3.1
1	B	2123	SER	3.1
1	B	1996	LEU	3.0
1	B	579	GLU	3.0
1	B	1858	ILE	2.9
1	B	1321	TYR	2.9
1	B	1876	PRO	2.9
1	B	1584	ILE	2.9
1	B	1859	PRO	2.8
1	B	567	ALA	2.8
1	B	1877	HIS	2.8
1	B	940	HIS	2.8
1	B	1968	SER	2.8
1	B	575	LEU	2.7
1	B	1307	LEU	2.7
1	B	405	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1955	SER	2.7
1	B	1261	PRO	2.7
2	J	2059	PRO	2.7
1	B	404	ALA	2.6
2	J	2157	VAL	2.6
1	B	576	CYS	2.6
1	B	1308	PRO	2.6
1	B	1600	TYR	2.5
1	B	1964	PRO	2.5
1	B	571	GLY	2.5
1	B	1170	MET	2.5
1	B	403	LEU	2.4
2	J	2061	GLY	2.4
1	B	859	PRO	2.4
1	B	1322	GLN	2.4
1	B	1849	ILE	2.4
1	B	1880	ASN	2.3
1	B	2027	ASP	2.3
1	B	1971	ILE	2.3
1	B	2107	TYR	2.3
1	B	1879	LEU	2.3
1	B	1998	GLN	2.3
1	B	1912	THR	2.2
1	B	1324	LYS	2.2
2	J	2100	THR	2.2
1	B	1882	PRO	2.2
1	B	1895	LEU	2.2
1	B	1842	VAL	2.2
1	B	943	LEU	2.2
1	B	1914	GLU	2.2
1	B	1136	PRO	2.1
2	J	2101	GLY	2.1
1	B	698	ILE	2.1
1	B	2051	VAL	2.1
1	B	2048	THR	2.1
1	B	1778	HIS	2.0
1	B	1966	PHE	2.0
1	B	1860	ILE	2.0
1	B	1982	VAL	2.0
1	B	1963	LEU	2.0
2	J	2320	LEU	2.0
1	B	570	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	J	2099	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](#)

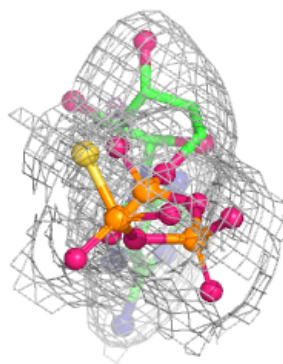
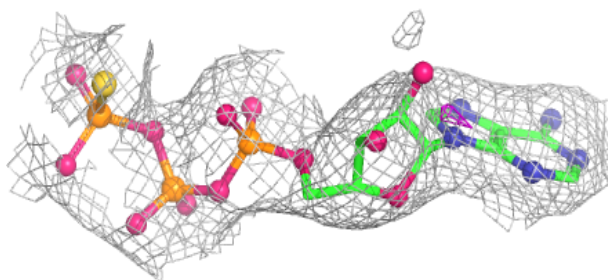
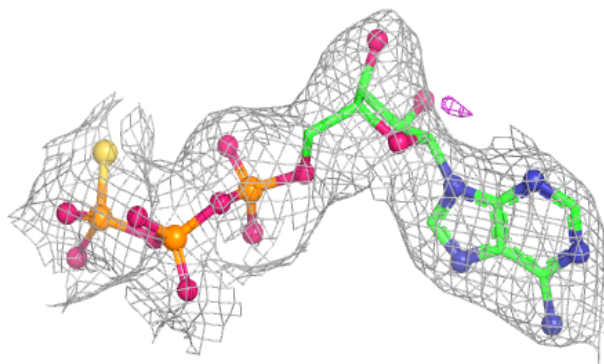
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	B	2203	1/1	0.90	0.18	53,53,53,53	0
4	MG	B	2204	1/1	0.94	0.12	46,46,46,46	0
3	AGS	B	2201	31/31	0.95	0.07	34,43,52,77	0
3	AGS	B	2202	31/31	0.95	0.07	35,51,61,61	0

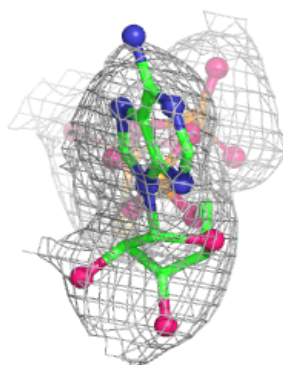
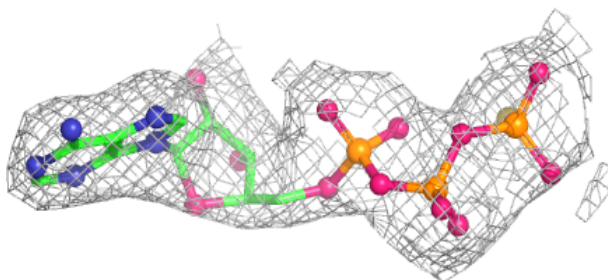
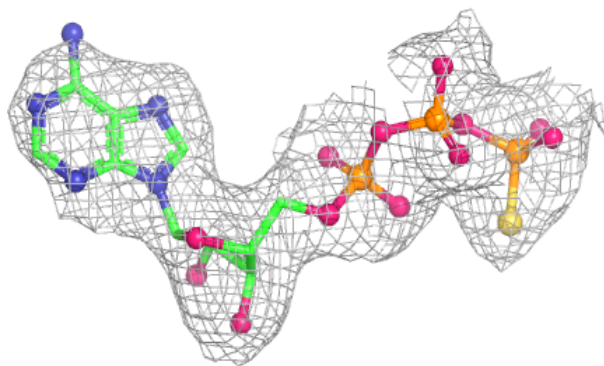
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS B 2201:

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

**Electron density around AGS 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.