



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:58 PM UTC

PDB ID : 4F93 / pdb_00004f93
Title : Brr2 Helicase Region S1087L, Mg-ATP
Authors : Santos, K.F.; Jovin, S.M.; Weber, G.; Pena, V.; Luehrmann, R.; Wahl, M.C.
Deposited on : 2012-05-18
Resolution : 2.92 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

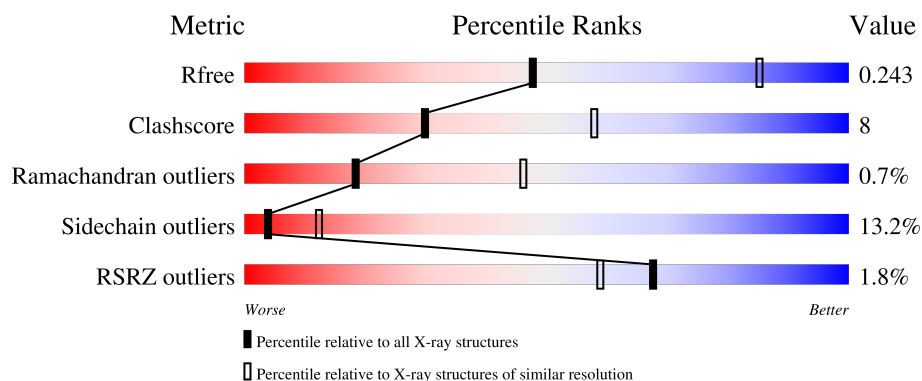
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	1724	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13987 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	1723	13866	8863	2373	2558	72	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1087	LEU	SER	engineered mutation	UNP O75643

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	27	10	5	10	2	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

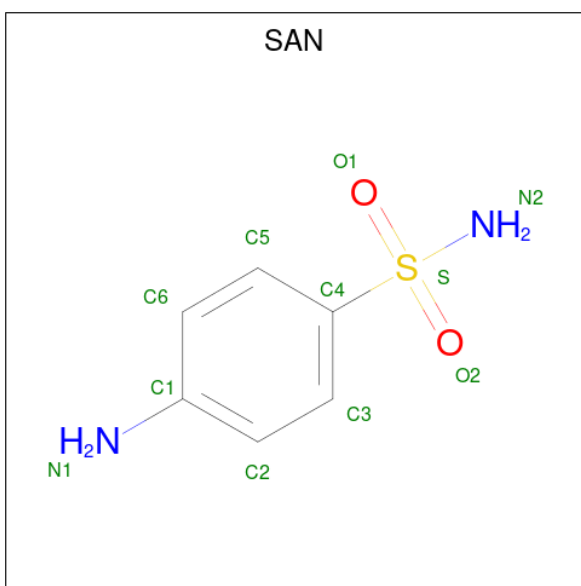


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is SULFANILAMIDE (CCD ID: SAN) (formula: $\text{C}_6\text{H}_8\text{N}_2\text{O}_2\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			11	6	2	2	1		

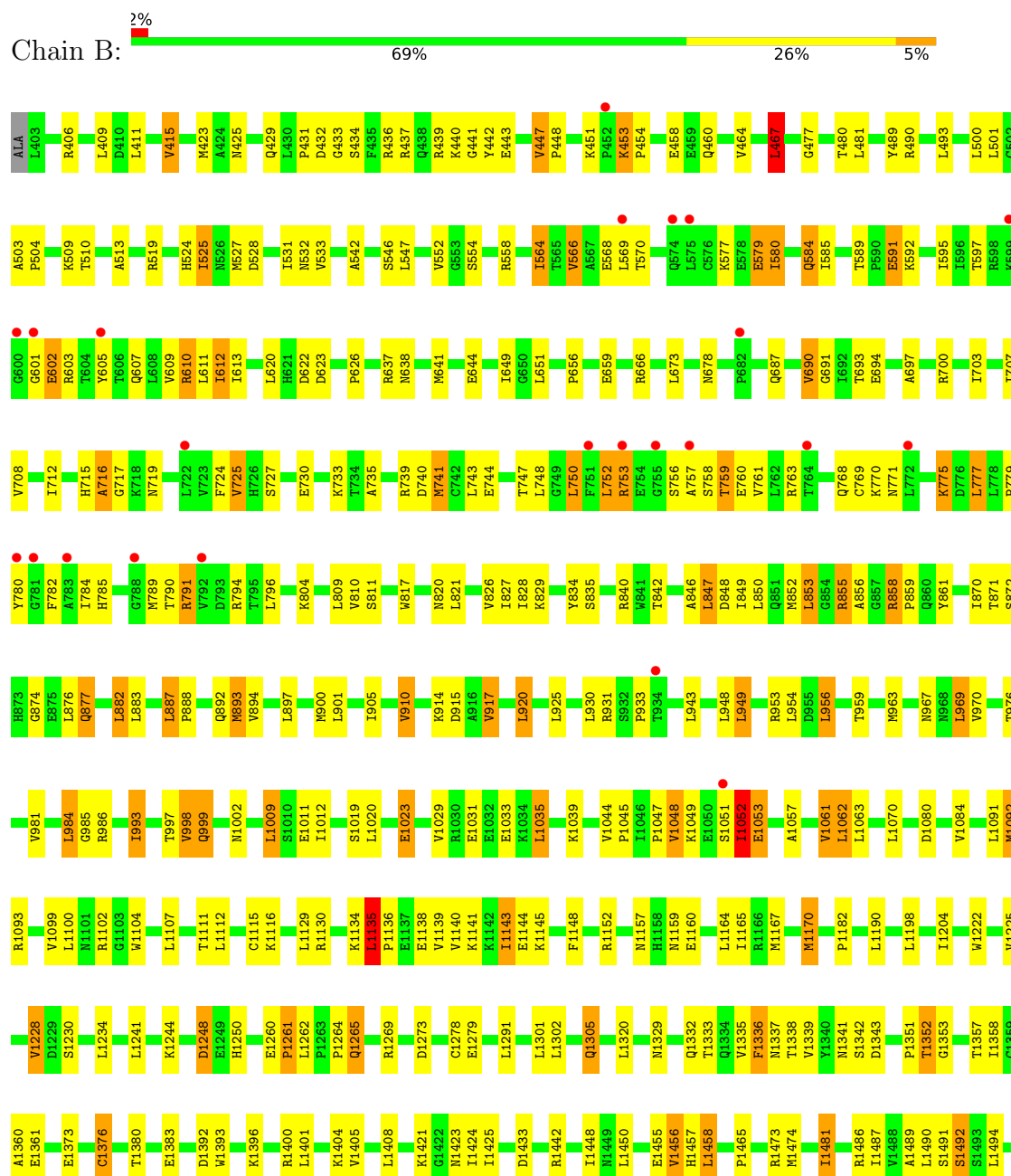
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	51	Total	O	0	0
			51	51		

3 Residue-property plots [i](#)

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

- Molecule 1: U5 small nuclear ribonucleoprotein 200 kDa helicase



K1498	L1809	T1742	A1853	G1978
A1501	K1610	K1743	E1854	V1979
H1502	E1611	T1744	Y1855	D1984
C1506	L1614	K1748	I1858	I1985
T1509	M1627	Q1749	P1859	M1986
P1516	F1636	D1753	I1860	N1994
N1517	S1637	T1756	R1861	A1995
V1518	V1644	R1763	L1871	L1996
R1519	S1649	Y1771	K1878	L1997
P1520	M1654	N1772	L1879	Q1998
V1521	L1773	Q1774	P1882	L1999
I1527	V1656	G1775	P1887	T2017
T1535	A1657	I1776	H1888	V2024
Q1536	A1658	S1777	T1891	D2025
T1537	D1665	H1778	L1894	K2026
R1538	L1672	R1779	L1895	T2029
L1539	Y1676	H1780	L1904	V2036
M1542	D1683	H1784	S1905	L2041
P1545	V1684	L1785	A1906	E2042
V1546	L1685	L1796	E1907	R2043
H1553	Q1686	E1797	L1908	A2053
T1560	M1687	I1802	D1911	P2054
T1569	V1688	S1803	L1922	L2055
L1577	G1689	I1804	L1937	F2056
C1580	M1692	M1808	P1938	P2057
A1581	R1693	M1814	M1943	R2060
A1582	P1694	I1818	E1944	V2067
D1583	Q1696	A1819	L1945	T2079
I1584	R1701	I1824	A1946	L2082
Q1585	M1705	N1825	Q1947	T2083
R1586	K1715	I1829	M1948	L2084
Q1587	L1718	E1830	V1949	K2087
R1588	L1722	L1831	T1950	K2091
F1589	E1725	M1834	W1954	L2092
L1590	L1728	T1840	S1955	T2099
T1593	L1734	K1841	K1956	C2116
E1594	D1739	V1842	L1960	D2117
K1595	I1740	L1845	L1963	Q2118
I1598	V1741	I1846	H1970	V2124
K1603	E1739	I1849	I1971	D2125
L1604	I1740	A1852	C1974	
S1607	V1741		K1977	
T1608				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.12Å 154.59Å 143.28Å 90.00° 120.62° 90.00°	Depositor
Resolution (Å)	47.36 – 2.92 47.36 – 2.92	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.36-2.92) 98.1 (47.36-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.197 , 0.248 (Not available) , 0.243	Depositor DCC
R_{free} test set	2926 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	88.6	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 113.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-1/2*h-1/2*k-l 0.000 for -k,-h,-1/2*h+1/2*k-l 0.003 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13987	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: SAN, ADP, ATP, 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	0.40	0/14161	0.85	25/19188 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1135	LEU	CA-C-N	7.29	128.95	119.84
1	B	1135	LEU	C-N-CA	7.29	128.95	119.84
1	B	757	ALA	N-CA-C	-7.21	105.67	114.75
1	B	877	GLN	N-CA-C	-6.86	104.91	113.28
1	B	2056	PHE	CA-C-N	6.42	126.11	119.56
1	B	2056	PHE	C-N-CA	6.42	126.11	119.56
1	B	1610	LYS	N-CA-C	-6.01	104.64	111.07
1	B	717	GLY	N-CA-C	5.98	119.73	112.49
1	B	1693	ARG	CA-C-N	5.72	126.11	119.47
1	B	1693	ARG	C-N-CA	5.72	126.11	119.47
1	B	1305	GLN	CA-C-N	5.72	125.73	119.90
1	B	1305	GLN	C-N-CA	5.72	125.73	119.90
1	B	835	SER	CA-C-N	5.50	124.96	119.24
1	B	835	SER	C-N-CA	5.50	124.96	119.24
1	B	750	LEU	N-CA-C	-5.39	106.20	112.89
1	B	2053	ALA	CA-C-N	5.31	126.48	119.84
1	B	2053	ALA	C-N-CA	5.31	126.48	119.84
1	B	467	LEU	CA-C-N	5.27	126.43	119.84
1	B	467	LEU	C-N-CA	5.27	126.43	119.84
1	B	1167	MET	CA-C-N	5.18	124.80	119.56
1	B	1167	MET	C-N-CA	5.18	124.80	119.56
1	B	2116	CYS	N-CA-C	-5.16	106.67	113.17
1	B	2084	LEU	N-CA-C	5.03	116.61	111.03
1	B	477	GLY	N-CA-C	-5.02	108.19	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	716	ALA	CB-CA-C	-5.02	110.40	117.23

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	13866	0	14008	237	0
2	B	27	0	12	2	0
3	B	31	0	12	0	0
4	B	1	0	0	0	0
5	B	11	0	8	0	0
6	B	51	0	0	7	0
All	All	13987	0	14040	237	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (237) 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:423:MET:HE3	1:B:425:ASN:HB3	1.58	0.84
1:B:993:ILE:HD11	1:B:998:VAL:HG23	1.60	0.84
1:B:1739:GLU:HG3	1:B:1744:THR:HB	1.61	0.82
1:B:1052:ILE:HG23	1:B:1053:GLU:H	1.56	0.70
1:B:1099:VAL:HG23	1:B:1104:TRP:HE3	1.57	0.70
1:B:933:PRO:HG3	1:B:943:LEU:HD22	1.74	0.69
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.73	0.69
1:B:715:HIS:HB3	1:B:719:ASN:HB3	1.72	0.69
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.74	0.68
1:B:930:LEU:HD23	1:B:949:LEU:HD22	1.76	0.68
1:B:997:THR:OG1	1:B:1023:GLU:OE1	2.09	0.68
1:B:610:ARG:HA	1:B:610:ARG:HH11	1.60	0.66
1:B:1099:VAL:HG23	1:B:1104:TRP:CE3	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1501:ALA:HB1	1:B:1506:CYS:HB2	1.80	0.64
1:B:641:MET:HA	1:B:1582:ALA:HB2	1.80	0.64
1:B:820:ASN:HA	1:B:855:ARG:HH12	1.61	0.64
1:B:1269:ARG:NH1	1:B:1279:GLU:OE2	2.30	0.64
1:B:759:THR:HG23	1:B:760:GLU:HG2	1.80	0.62
1:B:1456:VAL:HG11	1:B:1489:ALA:HB1	1.79	0.62
1:B:716:ALA:HB1	1:B:752:LEU:HD22	1.80	0.61
1:B:1433:ASP:OD2	1:B:1473:ARG:NH2	2.34	0.61
1:B:739:ARG:HG2	1:B:750:LEU:HD21	1.82	0.61
1:B:967:ASN:HA	1:B:999:GLN:HG2	1.83	0.60
1:B:984:LEU:HD21	1:B:1002:ASN:HB2	1.83	0.60
1:B:1861:ARG:NH1	1:B:1911:ASP:OD2	2.35	0.60
1:B:611:LEU:HD11	1:B:649:ILE:HD12	1.84	0.59
1:B:566:VAL:HB	1:B:585:ILE:HB	1.85	0.59
1:B:1456:VAL:HG22	1:B:1491:SER:HB2	1.84	0.58
1:B:1376:CYS:HB2	1:B:1450:LEU:HB3	1.84	0.58
1:B:2067:VAL:HG22	1:B:2079:ILE:HG13	1.85	0.58
1:B:796:LEU:HB3	6:B:3118:HOH:O	2.04	0.58
1:B:790:THR:HG23	1:B:794:ARG:HB2	1.84	0.58
1:B:1553:HIS:O	1:B:1701:ARG:NH1	2.30	0.57
1:B:603:ARG:O	1:B:607:GLN:HB2	2.03	0.57
1:B:1560:ILE:HD11	1:B:1656:VAL:HG12	1.86	0.57
1:B:724:PHE:CE2	1:B:852:MET:HB2	2.40	0.57
1:B:1457:HIS:CE1	1:B:1492:SER:HB2	2.39	0.57
1:B:725:VAL:HG13	1:B:829:LYS:HB3	1.86	0.57
1:B:597:THR:HA	1:B:602:GLU:HG3	1.86	0.57
1:B:525:ILE:HD13	1:B:525:ILE:H	1.68	0.57
1:B:777:LEU:HD12	1:B:782:PHE:HB2	1.88	0.56
1:B:1852:ALA:HB1	1:B:1854:GLU:HG2	1.86	0.56
1:B:1009:LEU:HB2	1:B:1107:LEU:HD22	1.87	0.56
1:B:1960:LEU:HD12	1:B:1971:ILE:HG23	1.88	0.56
1:B:1260:GLU:HB3	1:B:1261:PRO:HD3	1.86	0.56
1:B:524:HIS:HB3	1:B:532:ASN:HB2	1.88	0.55
1:B:910:VAL:HB	1:B:915:ASP:HB3	1.88	0.55
1:B:893:MET:HE1	1:B:900:MET:HG3	1.87	0.55
1:B:1607:SER:N	6:B:3116:HOH:O	2.39	0.55
1:B:564:ILE:HG12	1:B:584:GLN:HG3	1.88	0.55
1:B:1685:LEU:HD11	1:B:1722:LEU:HD22	1.89	0.55
1:B:1361:GLU:OE2	1:B:1393:TRP:NE1	2.32	0.55
1:B:1855:TYR:HA	1:B:1858:ILE:HD13	1.89	0.55
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.88	0.54
1:B:1970:HIS:HD2	1:B:1997:LEU:HD13	1.72	0.54
1:B:1057:ALA:O	1:B:1061:VAL:HG13	2.07	0.54
1:B:984:LEU:HG	1:B:998:VAL:HG13	1.90	0.54
1:B:2024:VAL:HB	1:B:2036:VAL:HB	1.90	0.54
1:B:1093:ARG:NH1	1:B:1273:ASP:OD2	2.41	0.54
1:B:1672:LYS:HD2	1:B:1887:PRO:HD3	1.90	0.54
1:B:948:LEU:O	1:B:953:ARG:NH1	2.42	0.53
1:B:1135:LEU:HD22	1:B:1136:PRO:HD2	1.90	0.53
1:B:1148:PHE:CZ	1:B:1152:ARG:HD2	2.42	0.53
1:B:554:SER:O	1:B:558:ARG:HG2	2.09	0.53
1:B:447:VAL:HG13	1:B:687:GLN:HG3	1.90	0.53
1:B:817:TRP:HH2	1:B:847:LEU:HD22	1.74	0.53
1:B:914:LYS:O	1:B:917:VAL:HG12	2.10	0.52
1:B:2043:ARG:HH11	1:B:2084:LEU:HD22	1.74	0.52
1:B:1950:THR:HG23	1:B:2060:ARG:HH12	1.73	0.52
1:B:1301:LEU:HD22	1:B:1518:VAL:HG13	1.90	0.52
1:B:1336:PHE:C	1:B:1336:PHE:CD2	2.87	0.52
1:B:442:TYR:HA	1:B:693:THR:HG23	1.92	0.52
1:B:504:PRO:HG3	1:B:678:ASN:HA	1.91	0.52
1:B:1373:GLU:HG3	1:B:1423:ASN:HD21	1.74	0.52
1:B:1604:LEU:HD13	1:B:1609:LEU:HD13	1.91	0.52
1:B:513:ALA:HB1	1:B:613:ILE:HD13	1.92	0.51
1:B:753:ARG:CG	1:B:753:ARG:HH21	2.22	0.51
1:B:1332:GLN:NE2	1:B:1358:ILE:HD11	2.26	0.51
1:B:1336:PHE:C	1:B:1336:PHE:HD2	2.19	0.51
1:B:1542:MET:C	1:B:1545:PRO:HD2	2.35	0.51
1:B:1609:LEU:HD12	6:B:3116:HOH:O	2.09	0.51
1:B:1796:LEU:HB3	1:B:1802:ILE:HG12	1.93	0.50
1:B:453:LYS:HG3	1:B:454:PRO:HD2	1.93	0.50
1:B:601:GLY:HA3	1:B:1537:THR:HG23	1.93	0.50
1:B:1228:VAL:HG13	1:B:1265:GLN:O	2.11	0.50
1:B:1262:LEU:HD11	1:B:1291:LEU:HD11	1.93	0.50
1:B:1855:TYR:HB3	1:B:1891:THR:HG21	1.93	0.50
1:B:1979:VAL:HG13	1:B:1984:ASP:HB2	1.93	0.50
1:B:1099:VAL:HG22	1:B:1104:TRP:HB2	1.92	0.50
1:B:1329:ASN:O	1:B:1333:THR:HG23	2.10	0.49
1:B:622:ASP:OD1	1:B:623:ASP:N	2.46	0.49
1:B:1352:THR:HG22	6:B:3113:HOH:O	2.13	0.49
1:B:436:ARG:NH1	1:B:443:GLU:OE2	2.45	0.49
1:B:1775:GLY:HA3	1:B:1780:HIS:CD2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:820:ASN:ND2	2:B:3001:ADP:O3'	2.46	0.49
1:B:1535:THR:HG21	1:B:1676:TYR:CE2	2.48	0.49
1:B:1846:ILE:HG23	1:B:1895:LEU:HD23	1.95	0.49
1:B:1905:SER:HB3	1:B:1908:LEU:HD12	1.94	0.49
1:B:1797:GLU:HG3	1:B:1804:ILE:HG13	1.95	0.48
1:B:626:PRO:HD3	1:B:892:GLN:HB2	1.95	0.48
1:B:513:ALA:HB2	1:B:651:LEU:HD11	1.96	0.48
1:B:1337:ASN:O	1:B:1341:ASN:HB2	2.14	0.48
1:B:1945:LEU:HA	1:B:1948:MET:HG2	1.96	0.48
1:B:1141:LYS:O	1:B:1145:LYS:HG2	2.13	0.48
1:B:1338:THR:O	1:B:1342:SER:HB2	2.13	0.48
1:B:1943:MET:HE1	1:B:2067:VAL:HG21	1.95	0.48
1:B:1392:ASP:O	1:B:1396:LYS:HB2	2.14	0.48
1:B:727:SER:HB2	1:B:730:GLU:HB2	1.96	0.48
1:B:1130:ARG:NE	1:B:1144:GLU:OE2	2.46	0.48
1:B:769:CYS:O	1:B:770:LYS:HD2	2.13	0.48
1:B:1580:CYS:SG	1:B:1588:ARG:HG2	2.54	0.48
1:B:1937:SER:HB2	1:B:1938:PRO:HD3	1.95	0.48
1:B:637:ARG:HD3	6:B:3131:HOH:O	2.14	0.48
1:B:2091:LYS:H	1:B:2091:LYS:HD3	1.78	0.48
1:B:874:GLY:HA2	6:B:3137:HOH:O	2.14	0.47
1:B:439:ARG:O	1:B:441:GLY:N	2.46	0.47
1:B:691:GLY:HA2	1:B:871:THR:O	2.14	0.47
1:B:1748:LYS:N	1:B:1808:MET:O	2.42	0.47
1:B:1819:ALA:HB2	1:B:1829:ILE:HG12	1.95	0.47
1:B:1248:ASP:O	1:B:1250:HIS:ND1	2.48	0.47
1:B:552:VAL:HG13	1:B:566:VAL:HG22	1.95	0.46
1:B:510:THR:HB	2:B:3001:ADP:O2A	2.16	0.46
1:B:2056:PHE:HA	1:B:2057:PRO:HD3	1.74	0.46
1:B:411:LEU:HD13	1:B:959:THR:HG21	1.97	0.46
1:B:834:TYR:OH	1:B:1080:ASP:OD1	2.18	0.46
1:B:1842:VAL:HA	1:B:1845:LEU:HD12	1.96	0.46
1:B:1970:HIS:CD2	1:B:1997:LEU:HD13	2.49	0.46
1:B:826:VAL:HG22	1:B:856:ALA:HB2	1.97	0.46
1:B:853:LEU:HD13	1:B:883:LEU:HD11	1.98	0.46
1:B:1683:ASP:O	1:B:1687:MET:HG3	2.16	0.46
1:B:1994:ASN:HB2	1:B:1999:LEU:HD13	1.96	0.46
1:B:1538:ARG:NH1	1:B:1665:ASP:OD2	2.48	0.46
1:B:690:VAL:HG13	1:B:870:ILE:HA	1.98	0.45
1:B:415:VAL:HG23	1:B:894:VAL:HB	1.98	0.45
1:B:1143:ILE:HB	1:B:1165:ILE:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1718:LEU:HD23	1:B:1718:LEU:HA	1.77	0.45
1:B:1753:ASP:O	1:B:1756:THR:OG1	2.23	0.45
1:B:785:HIS:HB3	1:B:811:SER:HB2	1.99	0.45
1:B:969:LEU:HD13	1:B:985:GLY:HA2	1.99	0.45
1:B:612:ILE:O	1:B:612:ILE:HG13	2.17	0.45
1:B:1481:ILE:HD13	1:B:1481:ILE:O	2.17	0.45
1:B:1986:MET:HE2	1:B:1986:MET:HA	1.98	0.45
1:B:872:SER:HB3	1:B:876:LEU:HD12	1.99	0.45
1:B:1035:LEU:HA	1:B:1035:LEU:HD23	1.78	0.45
1:B:1455:GLU:HB3	1:B:1458:LEU:HD23	1.97	0.45
1:B:2042:GLU:HG3	1:B:2087:LYS:HG2	1.98	0.45
1:B:790:THR:CG2	1:B:794:ARG:HB2	2.44	0.45
1:B:828:ILE:HD12	1:B:853:LEU:HD12	1.99	0.45
1:B:480:THR:OG1	1:B:481:LEU:N	2.50	0.45
1:B:1264:PRO:C	1:B:1265:GLN:HG3	2.42	0.44
1:B:784:ILE:HG22	1:B:810:VAL:HG13	1.99	0.44
1:B:1044:VAL:HA	1:B:1045:PRO:HD3	1.70	0.44
1:B:489:TYR:CZ	1:B:490:ARG:HG3	2.52	0.44
1:B:1107:LEU:O	1:B:1111:THR:OG1	2.30	0.44
1:B:1527:ILE:HD12	1:B:1715:LYS:HG2	2.00	0.44
1:B:735:ALA:HB2	1:B:810:VAL:CG1	2.48	0.44
1:B:1339:VAL:HA	1:B:1486:ARG:HH22	1.82	0.44
1:B:1636:PHE:CD1	1:B:1644:VAL:HG13	2.53	0.44
1:B:610:ARG:NH2	1:B:644:GLU:HB3	2.33	0.44
1:B:703:ILE:O	1:B:707:ILE:HG13	2.17	0.44
1:B:1603:LYS:O	1:B:1627:MET:HE1	2.18	0.44
1:B:1542:MET:HE2	1:B:1705:MET:HB3	2.00	0.44
1:B:1824:ILE:HD13	1:B:1922:LEU:HD23	2.00	0.44
1:B:591:GLU:O	1:B:595:ILE:HG13	2.18	0.44
1:B:1157:ASN:HB3	1:B:1160:GLU:OE1	2.17	0.44
1:B:1627:MET:HE3	1:B:1627:MET:HB3	1.93	0.44
1:B:464:VAL:HG13	1:B:467:LEU:HD22	1.99	0.43
1:B:569:LEU:O	1:B:592:LYS:HG2	2.18	0.43
1:B:759:THR:C	1:B:761:VAL:H	2.26	0.43
1:B:1948:MET:HE3	1:B:1954:TRP:HA	2.00	0.43
1:B:740:ASP:O	1:B:744:GLU:HG3	2.18	0.43
1:B:1062:LEU:HD13	1:B:1062:LEU:HA	1.84	0.43
1:B:411:LEU:HD22	1:B:963:MET:HE1	2.00	0.43
1:B:741:MET:HE2	1:B:741:MET:HB2	1.69	0.43
1:B:1693:ARG:HA	1:B:1694:PRO:HD2	1.85	0.43
1:B:775:LYS:NZ	1:B:775:LYS:HB3	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:848:ASP:O	1:B:852:MET:HG2	2.19	0.43
1:B:1776:ILE:HG13	1:B:1780:HIS:CE1	2.54	0.43
1:B:1773:LEU:HD22	1:B:1784:HIS:CG	2.54	0.43
1:B:708:VAL:O	1:B:712:ILE:HG13	2.18	0.43
1:B:846:ALA:HA	1:B:882:LEU:HD11	2.00	0.43
1:B:577:LYS:HB2	1:B:579:GLU:HG3	2.01	0.43
1:B:920:LEU:HD12	1:B:920:LEU:HA	1.70	0.43
1:B:503:ALA:HB3	1:B:509:LYS:HE3	2.00	0.43
1:B:1048:VAL:HG23	1:B:1051:SER:HB2	2.01	0.43
1:B:580:ILE:HD11	1:B:605:TYR:HD2	1.84	0.42
1:B:656:PRO:HB2	1:B:888:PRO:HA	2.00	0.42
1:B:1352:THR:OG1	1:B:1689:GLY:HA3	2.19	0.42
1:B:1672:LYS:HD3	1:B:1860:ILE:HG12	2.01	0.42
1:B:1139:VAL:HG21	1:B:1170:MET:HG2	2.00	0.42
1:B:1974:CYS:HA	1:B:1977:LYS:HB3	2.01	0.42
1:B:1351:PRO:CG	1:B:1516:PRO:HA	2.45	0.42
1:B:1852:ALA:O	1:B:1888:HIS:HE1	2.03	0.42
1:B:570:THR:HA	1:B:592:LYS:HG2	2.02	0.42
1:B:821:LEU:HD12	1:B:821:LEU:O	2.20	0.42
1:B:1603:LYS:HB2	1:B:1603:LYS:HE3	1.92	0.42
1:B:858:ARG:HA	1:B:859:PRO:HD3	1.87	0.42
1:B:1814:ASN:O	1:B:1818:ILE:HG23	2.20	0.42
1:B:1031:GLU:C	1:B:1033:GLU:H	2.28	0.42
1:B:1944:GLU:O	1:B:1947:GLN:HG2	2.19	0.42
1:B:1182:PRO:HB2	1:B:1278:CYS:SG	2.59	0.41
1:B:1582:ALA:C	1:B:1584:ILE:H	2.27	0.41
1:B:1891:THR:O	1:B:1895:LEU:HB2	2.20	0.41
1:B:791:ARG:HD3	1:B:791:ARG:HA	1.88	0.41
1:B:1092:MET:HB3	1:B:1115:CYS:SG	2.60	0.41
1:B:1404:LYS:HG2	1:B:1421:LYS:HE2	2.01	0.41
1:B:1740:ILE:HD12	1:B:1802:ILE:HG21	2.02	0.41
1:B:433:GLY:HA3	1:B:448:PRO:HD3	2.02	0.41
1:B:840:ARG:HE	1:B:842:THR:CG2	2.34	0.41
1:B:1112:LEU:HG	1:B:1116:LYS:HE2	2.01	0.41
1:B:1539:LEU:HD12	1:B:1539:LEU:HA	1.94	0.41
1:B:1734:ASP:OD2	1:B:1825:ASN:ND2	2.53	0.41
1:B:1725:GLU:HB3	1:B:1771:TYR:OH	2.20	0.41
1:B:542:ALA:O	1:B:589:THR:HA	2.21	0.41
1:B:609:VAL:O	1:B:610:ARG:NH1	2.53	0.41
1:B:656:PRO:HD2	1:B:887:LEU:O	2.21	0.41
1:B:768:GLN:HG3	1:B:779:PRO:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:ILE:HD13	1:B:852:MET:HE3	2.03	0.41
1:B:858:ARG:HH11	1:B:861:TYR:HB2	1.86	0.41
1:B:1012:ILE:HG12	1:B:1047:PRO:HG2	2.03	0.41
1:B:1222:TRP:NE1	1:B:1273:ASP:OD2	2.53	0.41
1:B:1763:ARG:HA	1:B:1763:ARG:HD2	1.82	0.41
1:B:451:LYS:HB2	1:B:451:LYS:HE3	1.86	0.41
1:B:429:GLN:O	1:B:429:GLN:HG3	2.21	0.40
1:B:493:LEU:O	1:B:519:ARG:NH2	2.52	0.40
1:B:697:ALA:HA	1:B:700:ARG:HB2	2.04	0.40
1:B:1519:ARG:HD3	1:B:1521:VAL:O	2.22	0.40
1:B:894:VAL:HG23	6:B:3106:HOH:O	2.20	0.40
1:B:1405:VAL:HG22	1:B:1424:ILE:HB	2.03	0.40
1:B:2017:ILE:HB	1:B:2118:GLN:NE2	2.37	0.40
1:B:659:GLU:H	1:B:659:GLU:CD	2.29	0.40
1:B:956:LEU:HD12	1:B:956:LEU:HA	1.93	0.40
1:B:1353:GLY:O	1:B:1692:ASN:ND2	2.55	0.40
1:B:579:GLU:HG3	1:B:579:GLU:H	1.65	0.40
1:B:777:LEU:HD13	1:B:777:LEU:HA	1.90	0.40
1:B:1894:LEU:HD21	1:B:1908:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1722/1724 (100%)	1603 (93%)	107 (6%)	12 (1%)	18 46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	756	SER
1	B	1049	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	758	SER
1	B	1052	ILE
1	B	1584	ILE
1	B	771	ASN
1	B	431	PRO
1	B	440	LYS
1	B	1882	PRO
1	B	780	TYR
1	B	747	THR
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	1543/1542 (100%)	1340 (87%)	203 (13%)	4 12

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	406	ARG
1	B	409	LEU
1	B	415	VAL
1	B	432	ASP
1	B	434	SER
1	B	437	ARG
1	B	447	VAL
1	B	453	LYS
1	B	458	GLU
1	B	460	GLN
1	B	467	LEU
1	B	500	LEU
1	B	501	LEU
1	B	525	ILE
1	B	527	MET
1	B	528	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	531	ILE
1	B	533	VAL
1	B	546	SER
1	B	547	LEU
1	B	564	ILE
1	B	566	VAL
1	B	568	GLU
1	B	579	GLU
1	B	580	ILE
1	B	584	GLN
1	B	591	GLU
1	B	602	GLU
1	B	610	ARG
1	B	612	ILE
1	B	620	LEU
1	B	638	ASN
1	B	666	ARG
1	B	673	LEU
1	B	690	VAL
1	B	694	GLU
1	B	725	VAL
1	B	733	LYS
1	B	741	MET
1	B	743	LEU
1	B	748	LEU
1	B	752	LEU
1	B	753	ARG
1	B	759	THR
1	B	763	ARG
1	B	775	LYS
1	B	777	LEU
1	B	789	MET
1	B	791	ARG
1	B	804	LYS
1	B	809	LEU
1	B	827	ILE
1	B	847	LEU
1	B	849	ILE
1	B	850	LEU
1	B	853	LEU
1	B	855	ARG
1	B	858	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	877	GLN
1	B	882	LEU
1	B	887	LEU
1	B	893	MET
1	B	897	LEU
1	B	901	LEU
1	B	910	VAL
1	B	917	VAL
1	B	920	LEU
1	B	925	LEU
1	B	931	ARG
1	B	949	LEU
1	B	954	LEU
1	B	956	LEU
1	B	969	LEU
1	B	970	VAL
1	B	976	THR
1	B	984	LEU
1	B	986	ARG
1	B	993	ILE
1	B	998	VAL
1	B	999	GLN
1	B	1009	LEU
1	B	1011	GLU
1	B	1019	SER
1	B	1020	LEU
1	B	1023	GLU
1	B	1029	VAL
1	B	1035	LEU
1	B	1039	LYS
1	B	1048	VAL
1	B	1052	ILE
1	B	1053	GLU
1	B	1061	VAL
1	B	1062	LEU
1	B	1063	LEU
1	B	1070	LEU
1	B	1084	VAL
1	B	1091	LEU
1	B	1092	MET
1	B	1100	LEU
1	B	1102	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1129	LEU
1	B	1134	LYS
1	B	1135	LEU
1	B	1138	GLU
1	B	1140	VAL
1	B	1143	ILE
1	B	1159	ASN
1	B	1164	LEU
1	B	1170	MET
1	B	1190	LEU
1	B	1198	LEU
1	B	1204	ILE
1	B	1225	VAL
1	B	1228	VAL
1	B	1230	SER
1	B	1234	LEU
1	B	1241	LEU
1	B	1244	LYS
1	B	1248	ASP
1	B	1265	GLN
1	B	1302	LEU
1	B	1305	GLN
1	B	1320	LEU
1	B	1335	VAL
1	B	1336	PHE
1	B	1343	ASP
1	B	1352	THR
1	B	1357	THR
1	B	1376	CYS
1	B	1380	THR
1	B	1383	GLU
1	B	1400	ARG
1	B	1401	LEU
1	B	1408	LEU
1	B	1425	ILE
1	B	1442	ARG
1	B	1448	ILE
1	B	1456	VAL
1	B	1458	LEU
1	B	1465	PRO
1	B	1474	MET
1	B	1481	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1487	ILE
1	B	1492	SER
1	B	1494	LEU
1	B	1498	LYS
1	B	1509	THR
1	B	1539	LEU
1	B	1546	VAL
1	B	1569	THR
1	B	1577	LEU
1	B	1586	ARG
1	B	1587	GLN
1	B	1590	LEU
1	B	1593	THR
1	B	1595	LYS
1	B	1598	ILE
1	B	1603	LYS
1	B	1609	LEU
1	B	1611	GLU
1	B	1614	LEU
1	B	1637	SER
1	B	1649	SER
1	B	1654	MET
1	B	1656	VAL
1	B	1672	LYS
1	B	1683	ASP
1	B	1692	ASN
1	B	1696	GLN
1	B	1728	LEU
1	B	1739	GLU
1	B	1741	VAL
1	B	1743	LYS
1	B	1749	GLN
1	B	1773	LEU
1	B	1776	ILE
1	B	1778	HIS
1	B	1785	LEU
1	B	1796	LEU
1	B	1818	ILE
1	B	1829	ILE
1	B	1831	LEU
1	B	1834	MET
1	B	1840	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1849	ILE
1	B	1854	GLU
1	B	1871	LEU
1	B	1878	LYS
1	B	1879	LEU
1	B	1904	LEU
1	B	1907	GLU
1	B	1956	LYS
1	B	1963	LEU
1	B	1996	LEU
1	B	2017	ILE
1	B	2026	LYS
1	B	2029	ILE
1	B	2041	LEU
1	B	2055	LEU
1	B	2082	LEU
1	B	2084	LEU
1	B	2092	LEU
1	B	2099	THR

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	726	HIS
1	B	785	HIS
1	B	805	HIS
1	B	820	ASN
1	B	884	ASN
1	B	902	ASN
1	B	911	GLN
1	B	918	ASN
1	B	1667	GLN
1	B	1707	GLN
1	B	1780	HIS
1	B	1784	HIS
1	B	1870	GLN
1	B	2040	GLN

5.3.3 RNA ⓘ

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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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$
5	SAN	B	3004	-	11,11,11	3.26	1 (9%)	16,16,16	2.22	4 (25%)
2	ADP	B	3001	-	28,29,29	1.49	5 (17%)	43,45,45	1.86	9 (20%)
3	ATP	B	3002	4	32,33,33	1.41	6 (18%)	48,52,52	1.75	9 (18%)

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
5	SAN	B	3004	-	-	4/6/6/6	0/1/1/1
2	ADP	B	3001	-	-	7/16/32/32	0/3/3/3
3	ATP	B	3002	4	-	5/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	3004	SAN	C4-S	-10.67	1.60	1.77
2	B	3001	ADP	C5-C4	4.78	1.47	1.39
3	B	3002	ATP	C5-C4	4.59	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3001	ADP	C5-C6	2.81	1.48	1.41
2	B	3001	ADP	PA-O3A	2.71	1.62	1.59
3	B	3002	ATP	C5-C6	2.65	1.48	1.41
2	B	3001	ADP	C8-N7	2.49	1.36	1.31
3	B	3002	ATP	C8-N7	2.32	1.36	1.31
3	B	3002	ATP	PA-O3A	2.27	1.61	1.59
2	B	3001	ADP	C5-N7	-2.22	1.35	1.39
3	B	3002	ATP	C5-N7	-2.20	1.35	1.39
3	B	3002	ATP	PB-O3A	2.15	1.61	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3004	SAN	O2-S-O1	-7.32	107.53	118.80
2	B	3001	ADP	C5-C4-N3	-6.02	118.42	126.72
3	B	3002	ATP	C5-C4-N3	-5.40	119.28	126.72
2	B	3001	ADP	N3-C4-N9	4.53	134.87	127.17
3	B	3002	ATP	N3-C4-N9	4.49	134.81	127.17
2	B	3001	ADP	C2-N3-C4	3.83	121.18	111.83
3	B	3002	ATP	C2-N3-C4	3.76	121.01	111.83
3	B	3002	ATP	N3-C2-N1	-3.65	123.06	128.58
2	B	3001	ADP	C4-C5-N7	-3.63	106.43	110.58
2	B	3001	ADP	N3-C2-N1	-3.30	123.59	128.58
3	B	3002	ATP	C4-C5-N7	-3.01	107.14	110.58
3	B	3002	ATP	C4-N9-C8	2.96	108.85	105.74
2	B	3001	ADP	O4'-C1'-N9	2.86	113.58	108.09
5	B	3004	SAN	O2-S-C4	2.74	110.45	107.35
2	B	3001	ADP	C5-N7-C8	2.58	107.51	103.45
3	B	3002	ATP	C5-N7-C8	2.38	107.19	103.45
2	B	3001	ADP	C6-C5-N7	2.24	136.40	132.09
3	B	3002	ATP	C6-C5-N7	2.16	136.25	132.09
2	B	3001	ADP	C4-N9-C8	2.16	108.00	105.74
5	B	3004	SAN	O1-S-N2	2.15	110.45	107.35
3	B	3002	ATP	N9-C8-N7	-2.13	110.91	113.94
5	B	3004	SAN	O1-S-C4	2.13	109.75	107.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3001	ADP	PA-O3A-PB-O2B
2	B	3001	ADP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	3001	ADP	C5'-O5'-PA-O2A
2	B	3001	ADP	C5'-O5'-PA-O3A
5	B	3004	SAN	C5-C4-S-N2
5	B	3004	SAN	C3-C4-S-N2
3	B	3002	ATP	C2'-C1'-N9-C8
2	B	3001	ADP	C4'-C5'-O5'-PA
5	B	3004	SAN	C5-C4-S-O1
5	B	3004	SAN	C3-C4-S-O1
2	B	3001	ADP	PA-O3A-PB-O3B
3	B	3002	ATP	PB-O3A-PA-O1A
2	B	3001	ADP	PA-O3A-PB-O1B
3	B	3002	ATP	O4'-C1'-N9-C8
3	B	3002	ATP	PA-O3A-PB-O2B
3	B	3002	ATP	PB-O3A-PA-O2A

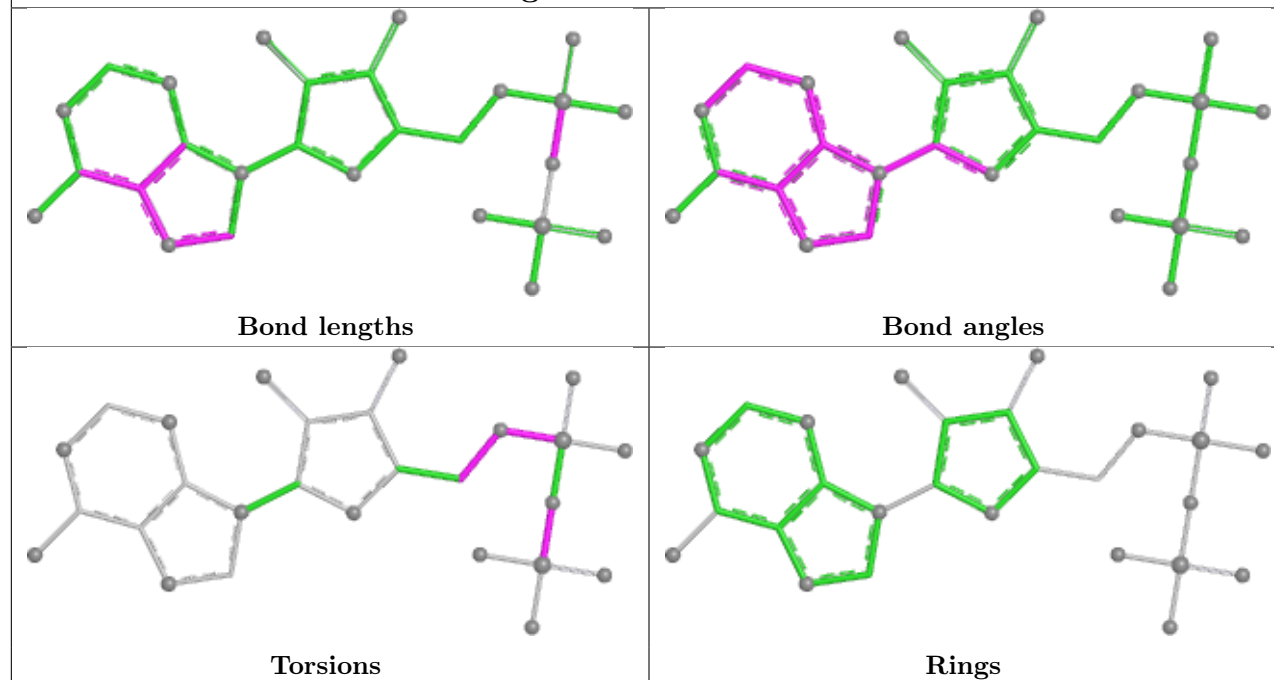
There are no ring outliers.

1 monomer is involved in 2 short contacts:

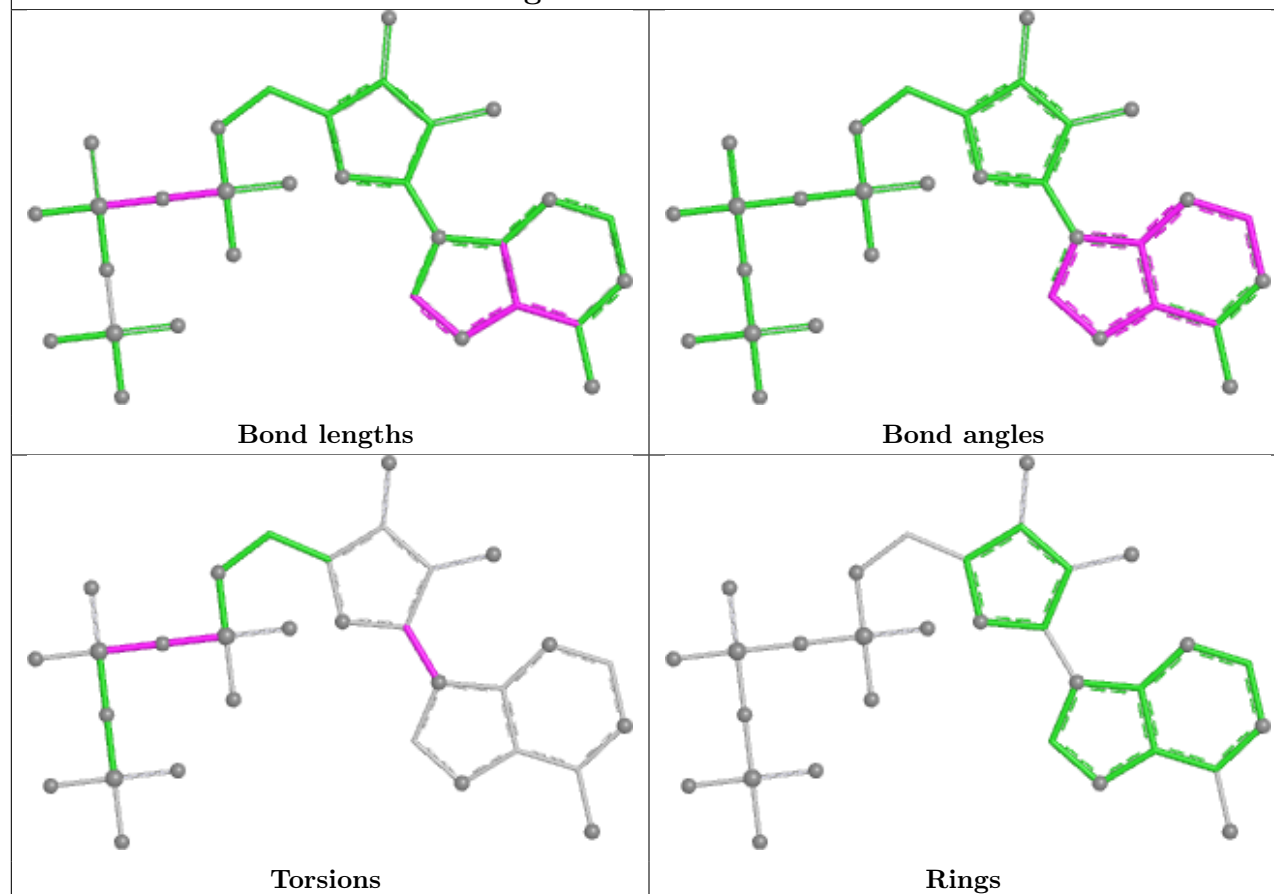
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3001	ADP	2	0

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.

Ligand ADP B 3001



Ligand ATP B 3002



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	1723/1724 (99%)	0.03	31 (1%) 67 59	62, 127, 213, 267	1 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1985	ILE	3.6
1	B	757	ALA	3.5
1	B	772	LEU	3.5
1	B	1776	ILE	3.4
1	B	1051	SER	3.3
1	B	722	LEU	3.2
1	B	783	ALA	3.2
1	B	575	LEU	3.0
1	B	601	GLY	2.9
1	B	569	LEU	2.9
1	B	781	GLY	2.8
1	B	452	PRO	2.6
1	B	2084	LEU	2.6
1	B	599	LYS	2.5
1	B	792	VAL	2.4
1	B	600	GLY	2.4
1	B	2124	VAL	2.4
1	B	751	PHE	2.4
1	B	788	GLY	2.3
1	B	605	TYR	2.3
1	B	1963	LEU	2.2
1	B	1502[A]	HIS	2.2
1	B	780	TYR	2.2
1	B	753	ARG	2.2
1	B	934	THR	2.1
1	B	764	THR	2.1
1	B	682	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	574	GLN	2.1
1	B	755	GLY	2.0
1	B	1979	VAL	2.0
1	B	1655	ASN	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](#)

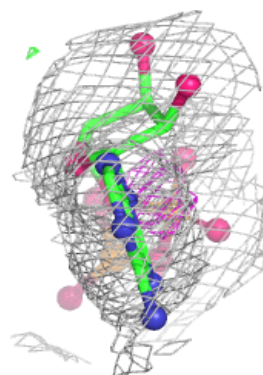
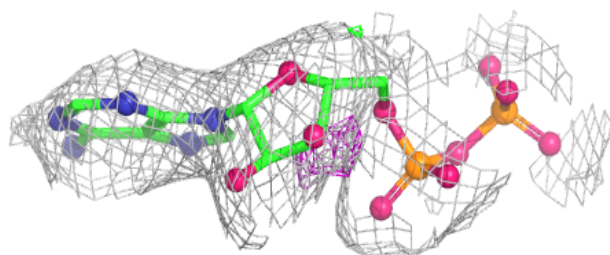
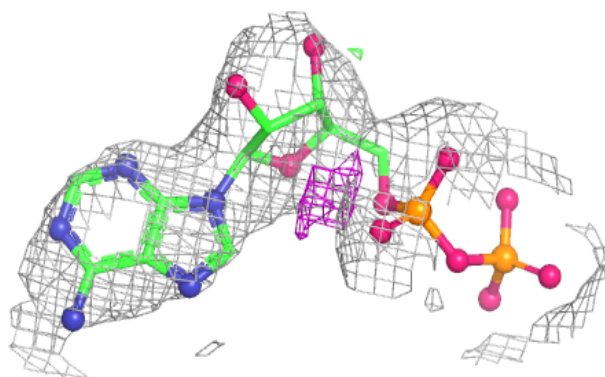
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	ADP	B	3001	27/27	0.91	0.09	116,145,168,183	0
3	ATP	B	3002	31/31	0.92	0.10	87,120,199,217	0
4	MG	B	3003	1/1	0.92	0.24	164,164,164,164	0
5	SAN	B	3004	11/11	0.93	0.12	96,102,121,132	0

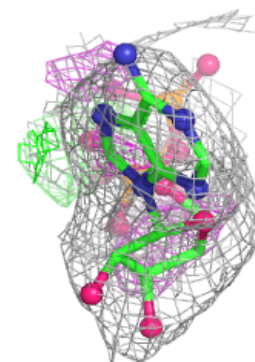
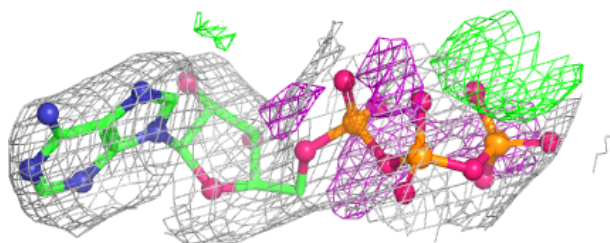
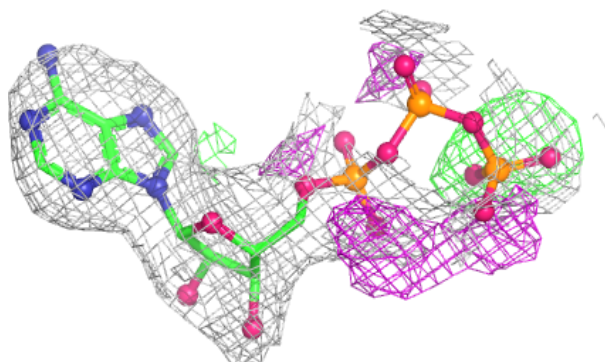
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 3001:

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

**Electron density around ATP B 3002:**

$2mF_o-DF_c$ (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.