



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:07 am GMT

PDB ID : 4F93
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

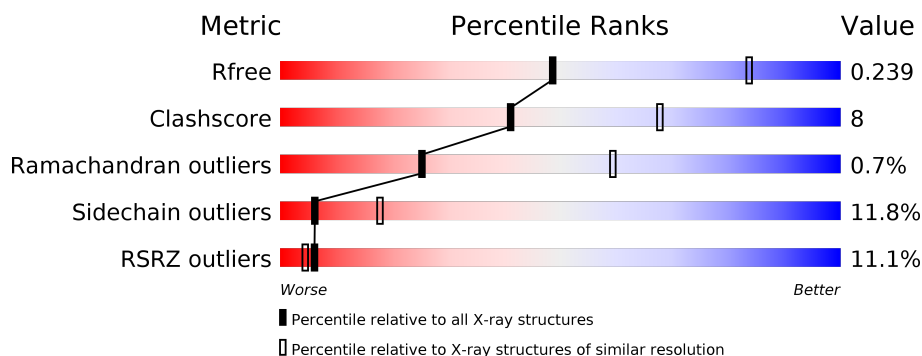
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

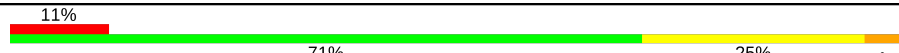
The reported resolution of this entry is 2.92 Å.

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}	100719	1813 (2.94-2.90)
Clashscore	112137	2045 (2.94-2.90)
Ramachandran outliers	110173	1997 (2.94-2.90)
Sidechain outliers	110143	1999 (2.94-2.90)
RSRZ outliers	101464	1825 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

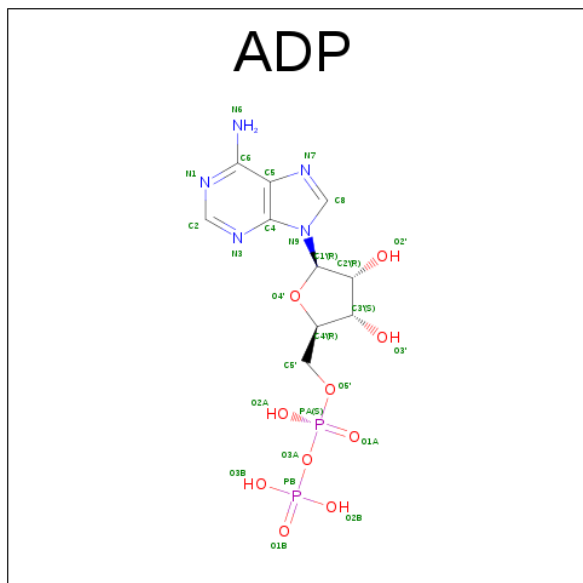
- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

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 (three-letter code: 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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

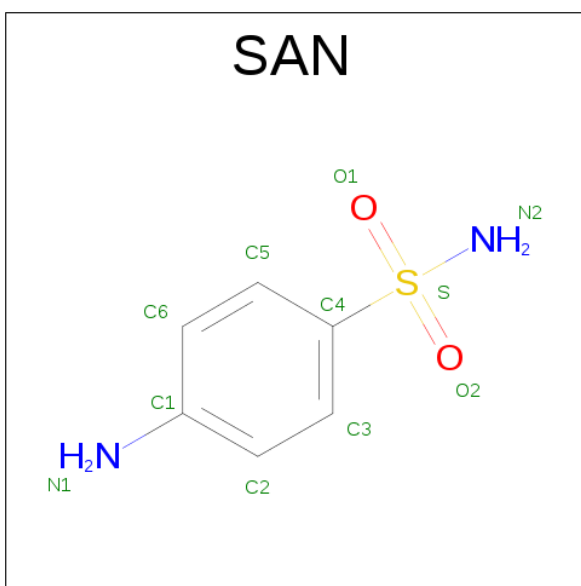


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is SULFANILAMIDE (three-letter code: 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		

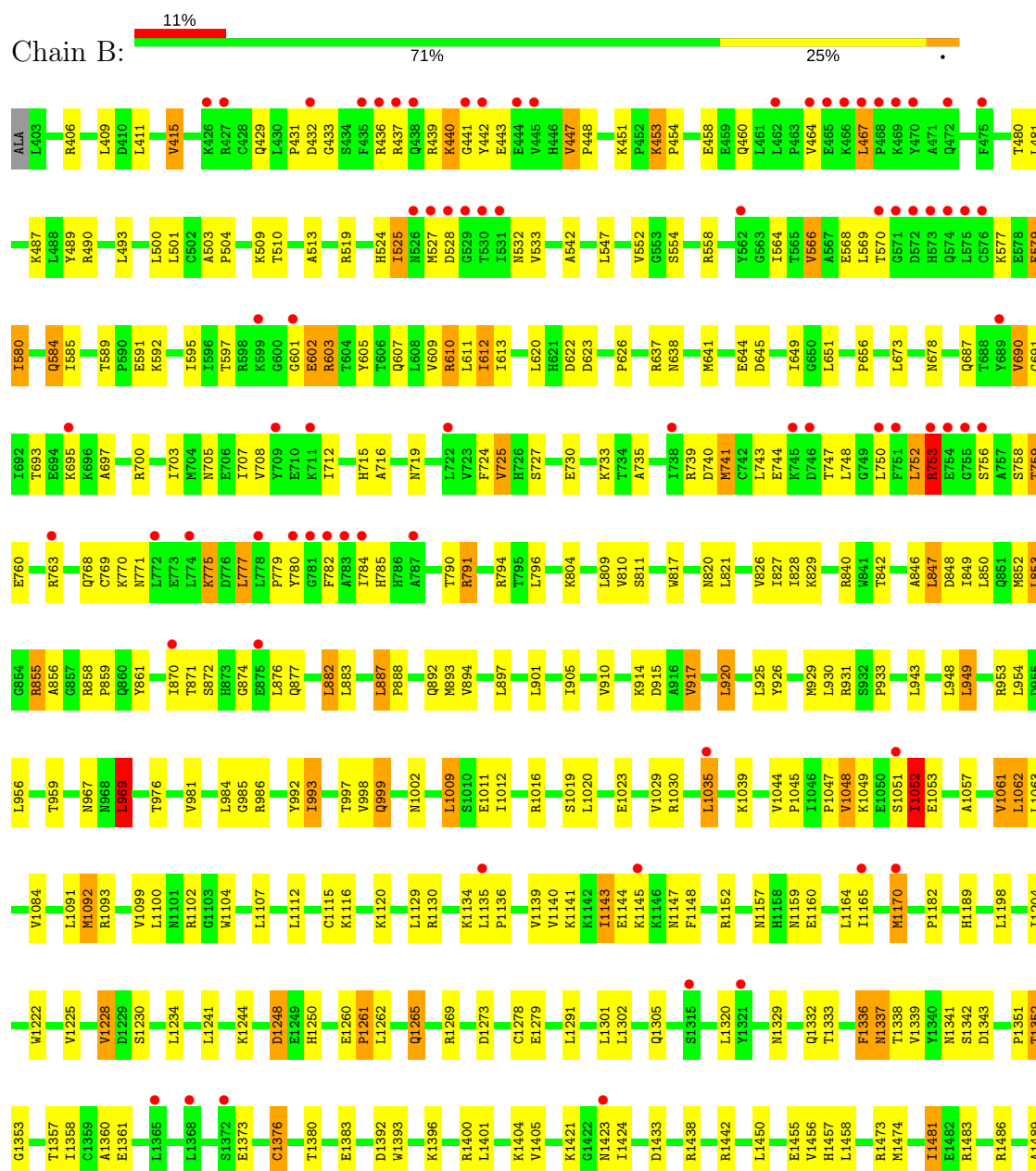
- Molecule 6 is water.

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

3 Residue-property plots

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

- Molecule 1: U5 small nuclear ribonucleoprotein 200 kDa helicase





4 Data and refinement statistics

Property	Value	Source
Space group	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 48.20 – 2.92	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.36-2.92) 98.2 (48.20-2.92)	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 0.185 , 0.239	Depositor DCC
R_{free} test set	2916 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	88.6	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.2	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: MG, ATP, ADP, SAN

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	0.31	0/14161	0.52	3/19188 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	969	LEU	CA-CB-CG	6.01	129.13	115.30
1	B	1609	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	753	ARG	NE-CZ-NH2	5.12	122.86	120.30

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	226	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	8	0
All	All	13987	0	14040	226	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 (226) 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: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:HH11	1:B:610:ARG:HA	1.60	0.66
1:B:1099:VAL:HG23	1:B:1104:TRP:CE3	2.31	0.66
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:1457:HIS:CE1	1:B:1492:SER:HB2	2.39	0.57
1:B:724:PHE:CE2	1:B:852:MET:HB2	2.40	0.57
1:B:725:VAL:HG13	1:B:829:LYS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:1970:HIS:HD2	1:B:1997:LEU:HD13	1.72	0.54
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.88	0.54
1:B:1057:ALA:O	1:B:1061:VAL:HG13	2.07	0.54
1:B:2024:VAL:HB	1:B:2036:VAL:HB	1.90	0.54
1:B:984:LEU:HG	1:B:998:VAL:HG13	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:1135:LEU:HD22	1:B:1136:PRO:HD2	1.90	0.53
1:B:948:LEU:O	1:B:953:ARG:NH1	2.42	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:442:TYR:HA	1:B:693:THR:HG23	1.92	0.52
1:B:1373:GLU:HG3	1:B:1423:ASN:HD21	1.74	0.52
1:B:504:PRO:HG3	1:B:678:ASN:HA	1.91	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:LYS:HG3	1:B:454:PRO:HD2	1.93	0.50
1:B:1228:VAL:HG13	1:B:1265:GLN:O	2.11	0.50
1:B:601:GLY:HA3	1:B:1537:THR:HG23	1.93	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:1352:THR:HG22	6:B:3113:HOH:O	2.13	0.49
1:B:622:ASP:OD1	1:B:623:ASP:N	2.46	0.49
1:B:1775:GLY:HA3	1:B:1780:HIS:CD2	2.48	0.49
1:B:436:ARG:NH1	1:B:443:GLU:OE2	2.45	0.49
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: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:513:ALA:HB2	1:B:651:LEU:HD11	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:1392:ASP:O	1:B:1396:LYS:HB2	2.14	0.48
1:B:1130:ARG:NE	1:B:1144:GLU:OE2	2.46	0.48
1:B:727:SER:HB2	1:B:730:GLU:HB2	1.96	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:2091:LYS:H	1:B:2091:LYS:HD3	1.78	0.48
1:B:637:ARG:HD3	6:B:3131:HOH:O	2.14	0.48
1:B:874:GLY:HA2	6:B:3137:HOH:O	2.14	0.47
1:B:1336:PHE:C	1:B:1336:PHE:CD2	2.87	0.47
1:B:439:ARG:O	1:B:441:GLY:N	2.46	0.47
1:B:1819:ALA:HB2	1:B:1829:ILE:HG12	1.95	0.47
1:B:1748:LYS:N	1:B:1808:MET:O	2.42	0.47
1:B:691:GLY:HA2	1:B:871:THR:O	2.14	0.47
1:B:1248:ASP:O	1:B:1250:HIS:ND1	2.48	0.47
1:B:705:ASN:HB3	1:B:741:MET:HE1	1.97	0.47
1:B:1336:PHE:C	1:B:1336:PHE:HD2	2.19	0.46
1:B:1542:MET:C	1:B:1545:PRO:HD2	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:VAL:HG13	1:B:566:VAL:HG22	1.95	0.46
1:B:2056:PHE:HA	1:B:2057:PRO:HD3	1.74	0.46
1:B:510:THR:HB	2:B:3001:ADP:O2A	2.16	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:411:LEU:HD13	1:B:959:THR:HG21	1.97	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
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:1481:ILE:HD13	1:B:1481:ILE:O	2.17	0.45
1:B:612:ILE:O	1:B:612:ILE:HG13	2.17	0.45
1:B:1035:LEU:HD23	1:B:1035:LEU:HA	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:872:SER:HB3	1:B:876:LEU:HD12	1.99	0.45
1:B:1627:MET:HE3	1:B:1627:MET:HB3	1.76	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:926:TYR:HA	1:B:929:MET:HE2	1.99	0.45
1:B:1044:VAL:HA	1:B:1045:PRO:HD3	1.70	0.44
1:B:784:ILE:HG22	1:B:810:VAL:HG13	1.99	0.44
1:B:489:TYR:CZ	1:B:490:ARG:HG3	2.52	0.44
1:B:1527:ILE:HD12	1:B:1715:LYS:HG2	2.00	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:735:ALA:HB2	1:B:810:VAL:CG1	2.48	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:1824:ILE:HD13	1:B:1922:LEU:HD23	2.00	0.44
1:B:1157:ASN:HB3	1:B:1160:GLU:OE1	2.17	0.44
1:B:591:GLU:O	1:B:595:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1062:LEU:HA	1:B:1062:LEU:HD13	1.84	0.43
1:B:740:ASP:O	1:B:744:GLU:HG3	2.18	0.43
1:B:1693:ARG:HA	1:B:1694:PRO:HD2	1.85	0.43
1:B:1776:ILE:HG13	1:B:1780:HIS:CE1	2.54	0.43
1:B:775:LYS:HB3	1:B:775:LYS:NZ	2.34	0.43
1:B:848:ASP:O	1:B:852:MET:HG2	2.19	0.43
1:B:1773:LEU:HD22	1:B:1784:HIS:CG	2.54	0.43
1:B:1948:MET:HE3	1:B:1954:TRP:HA	2.00	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:1048:VAL:HG23	1:B:1051:SER:HB2	2.01	0.43
1:B:503:ALA:HB3	1:B:509:LYS:HE3	2.00	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:1603:LYS:HE3	1:B:1603:LYS:HB2	1.92	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:1814:ASN:O	1:B:1818:ILE:HG23	2.20	0.42
1:B:858:ARG:HA	1:B:859:PRO:HD3	1.87	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: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:1189:HIS:ND1	6:B:3135:HOH:O	2.37	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:1112:LEU:HG	1:B:1116:LYS:HE2	2.01	0.41
1:B:1539:LEU:HA	1:B:1539:LEU:HD12	1.94	0.41
1:B:1734:ASP:OD2	1:B:1825:ASN:ND2	2.53	0.41
1:B:433:GLY:HA3	1:B:448:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:840:ARG:HE	1:B:842:THR:CG2	2.34	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:429:GLN:O	1:B:429:GLN:HG3	2.21	0.41
1:B:768:GLN:HG3	1:B:779:PRO:HG3	2.03	0.41
1:B:656:PRO:HD2	1:B:887:LEU:O	2.21	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:HD2	1:B:1763:ARG:HA	1.82	0.41
1:B:858:ARG:HH11	1:B:861:TYR:HB2	1.86	0.41
1:B:451:LYS:HB2	1:B:451:LYS:HE3	1.86	0.41
1:B:1519:ARG:HD3	1:B:1521:VAL:O	2.22	0.40
1:B:1729:ASP:N	1:B:1729:ASP:OD1	2.55	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:1405:VAL:HG22	1:B:1424:ILE:HB	2.03	0.40
1:B:1953:MET:HE3	1:B:1961:LYS:HB2	2.03	0.40
1:B:2017:ILE:HB	1:B:2118:GLN:NE2	2.37	0.40
1:B:894:VAL:HG23	6:B:3106:HOH:O	2.20	0.40
1:B:956:LEU:HA	1:B:956:LEU:HD12	1.93	0.40
1:B:1353:GLY:O	1:B:1692:ASN:ND2	2.55	0.40
1:B:1894:LEU:HD21	1:B:1908:LEU:HD22	2.03	0.40
1:B:579:GLU:H	1:B:579:GLU:HG3	1.65	0.40
1:B:777:LEU:HD13	1:B:777:LEU:HA	1.90	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	1722/1724 (100%)	1603 (93%)	107 (6%)	12 (1%)	25 59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	756	SER
1	B	1049	LYS
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%)	1361 (88%)	182 (12%)	6 18

All (182) 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	437	ARG
1	B	440	LYS
1	B	447	VAL
1	B	453	LYS
1	B	458	GLU
1	B	460	GLN
1	B	467	LEU
1	B	487	LYS
1	B	500	LEU

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Mol	Chain	Res	Type
1	B	501	LEU
1	B	525	ILE
1	B	527	MET
1	B	528	ASP
1	B	533	VAL
1	B	547	LEU
1	B	566	VAL
1	B	568	GLU
1	B	579	GLU
1	B	580	ILE
1	B	584	GLN
1	B	602	GLU
1	B	603	ARG
1	B	610	ARG
1	B	612	ILE
1	B	620	LEU
1	B	638	ASN
1	B	645	ASP
1	B	673	LEU
1	B	690	VAL
1	B	695	LYS
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	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	877	GLN

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Mol	Chain	Res	Type
1	B	882	LEU
1	B	887	LEU
1	B	893	MET
1	B	897	LEU
1	B	901	LEU
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	969	LEU
1	B	976	THR
1	B	986	ARG
1	B	992	TYR
1	B	993	ILE
1	B	999	GLN
1	B	1009	LEU
1	B	1011	GLU
1	B	1016	ARG
1	B	1019	SER
1	B	1020	LEU
1	B	1029	VAL
1	B	1030	ARG
1	B	1035	LEU
1	B	1039	LYS
1	B	1048	VAL
1	B	1052	ILE
1	B	1061	VAL
1	B	1062	LEU
1	B	1063	LEU
1	B	1084	VAL
1	B	1091	LEU
1	B	1092	MET
1	B	1100	LEU
1	B	1102	ARG
1	B	1120	LYS
1	B	1129	LEU
1	B	1134	LYS
1	B	1140	VAL
1	B	1143	ILE
1	B	1147	ASN

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Mol	Chain	Res	Type
1	B	1159	ASN
1	B	1164	LEU
1	B	1170	MET
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	1336	PHE
1	B	1337	ASN
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	1438	ARG
1	B	1442	ARG
1	B	1474	MET
1	B	1481	ILE
1	B	1483	ARG
1	B	1492	SER
1	B	1494	LEU
1	B	1498	LYS
1	B	1509	THR
1	B	1539	LEU
1	B	1569	THR
1	B	1577	LEU
1	B	1586	ARG
1	B	1587	GLN
1	B	1590	LEU
1	B	1593	THR

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Mol	Chain	Res	Type
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	1672	LYS
1	B	1683	ASP
1	B	1692	ASN
1	B	1696	GLN
1	B	1699	GLU
1	B	1728	LEU
1	B	1731	CYS
1	B	1739	GLU
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	1800	LYS
1	B	1818	ILE
1	B	1831	LEU
1	B	1834	MET
1	B	1840	THR
1	B	1849	ILE
1	B	1871	LEU
1	B	1878	LYS
1	B	1879	LEU
1	B	1904	LEU
1	B	1907	GLU
1	B	1928	ASP
1	B	1996	LEU
1	B	2026	LYS
1	B	2041	LEU
1	B	2055	LEU
1	B	2082	LEU
1	B	2084	LEU
1	B	2091	LYS
1	B	2092	LEU

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Mol	Chain	Res	Type
1	B	2099	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	820	ASN
1	B	1655	ASN
1	B	1862	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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$
2	ADP	B	3001	-	25,29,29	1.05	2 (8%)	24,45,45	1.67	2 (8%)
3	ATP	B	3002	4	27,33,33	0.99	1 (3%)	25,52,52	1.72	2 (8%)
5	SAN	B	3004	-	11,11,11	2.99	1 (9%)	16,16,16	1.92	3 (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
2	ADP	B	3001	-	-	0/12/32/32	0/3/3/3
3	ATP	B	3002	4	-	0/18/38/38	0/3/3/3
5	SAN	B	3004	-	-	0/6/6/6	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	3004	SAN	C4-S	-9.76	1.60	1.77
2	B	3001	ADP	O4'-C1'	2.07	1.44	1.41
3	B	3002	ATP	C5-C4	3.00	1.47	1.40
2	B	3001	ADP	C5-C4	3.15	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3002	ATP	N3-C2-N1	-6.65	123.06	128.86
5	B	3004	SAN	O2-S-O1	-6.09	107.53	118.70
2	B	3001	ADP	N3-C2-N1	-6.05	123.59	128.86
2	B	3001	ADP	C4-C5-N7	-3.09	106.43	109.41
3	B	3002	ATP	C4-C5-N7	-2.35	107.14	109.41
5	B	3004	SAN	O1-S-C4	2.02	109.75	107.39
5	B	3004	SAN	O2-S-C4	2.61	110.45	107.39

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.56	191 (11%) 6 4	66, 127, 213, 267	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2084	LEU	8.4
1	B	1963	LEU	8.0
1	B	2019	LEU	7.3
1	B	1985	ILE	7.3
1	B	751	PHE	7.1
1	B	1982	VAL	6.7
1	B	1971	ILE	6.5
1	B	1980	GLU	6.4
1	B	2038	LEU	6.3
1	B	2035	VAL	6.3
1	B	2124	VAL	6.3
1	B	2017	ILE	6.2
1	B	1960	LEU	6.2
1	B	1981	SER	6.0
1	B	1979	VAL	6.0
1	B	1988	MET	5.9
1	B	1991	GLU	5.8
1	B	781	GLY	5.7
1	B	2016	ASN	5.7
1	B	527	MET	5.6
1	B	2037	VAL	5.5
1	B	466	LYS	5.5
1	B	2036	VAL	5.5
1	B	572	ASP	5.5
1	B	571	GLY	5.2
1	B	574	GLN	5.2
1	B	573	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	528	ASP	5.0
1	B	2087	LYS	5.0
1	B	2015	PRO	4.9
1	B	2022	GLU	4.9
1	B	1968	SER	4.9
1	B	2113	TYR	4.8
1	B	1983	PHE	4.6
1	B	1987	GLU	4.6
1	B	1872	ALA	4.5
1	B	780	TYR	4.5
1	B	2010	PHE	4.5
1	B	1977	LYS	4.5
1	B	2106	LEU	4.5
1	B	1972	LYS	4.5
1	B	1964	PRO	4.5
1	B	1996	LEU	4.4
1	B	2039	VAL	4.4
1	B	1969	GLU	4.4
1	B	1976	ASP	4.3
1	B	1986	MET	4.3
1	B	1993	ARG	4.3
1	B	427	ARG	4.3
1	B	2104	TYR	4.3
1	B	783	ALA	4.2
1	B	754	GLU	4.1
1	B	1975	THR	4.0
1	B	1978	GLY	4.0
1	B	2085	GLN	4.0
1	B	2014	TYR	4.0
1	B	2120	TYR	4.0
1	B	531	ILE	3.9
1	B	1962	GLN	3.9
1	B	1365	LEU	3.9
1	B	2024	VAL	3.9
1	B	1989	GLU	3.8
1	B	756	SER	3.8
1	B	1868	LEU	3.8
1	B	2052	ILE	3.8
1	B	2098	ALA	3.7
1	B	782	PHE	3.7
1	B	2044	GLU	3.7
1	B	435	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	530	THR	3.7
1	B	755	GLY	3.6
1	B	1961	LYS	3.6
1	B	469	LYS	3.6
1	B	2041	LEU	3.6
1	B	722	LEU	3.5
1	B	470	TYR	3.5
1	B	426	LYS	3.5
1	B	745	LYS	3.5
1	B	2008	ALA	3.5
1	B	2018	GLU	3.4
1	B	2108	PHE	3.4
1	B	2043	ARG	3.4
1	B	1959	TYR	3.4
1	B	1873	GLN	3.3
1	B	1372	SER	3.3
1	B	1966	PHE	3.3
1	B	436	ARG	3.3
1	B	465	GLU	3.3
1	B	437	ARG	3.3
1	B	1997	LEU	3.2
1	B	2047	VAL	3.2
1	B	1974	CYS	3.2
1	B	1774	GLN	3.2
1	B	763	ARG	3.2
1	B	576	CYS	3.1
1	B	2102	HIS	3.1
1	B	2066	VAL	3.1
1	B	2086	GLN	3.1
1	B	2119	GLU	3.1
1	B	1879	LEU	3.0
1	B	1165	ILE	3.0
1	B	570	THR	3.0
1	B	1884	PHE	3.0
1	B	2112	ALA	2.9
1	B	695	LYS	2.9
1	B	467	LEU	2.9
1	B	1995	ALA	2.9
1	B	1051	SER	2.9
1	B	2118	GLN	2.9
1	B	442	TYR	2.9
1	B	711	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	526	ASN	2.9
1	B	1973	ARG	2.8
1	B	1871	LEU	2.8
1	B	2122	PHE	2.8
1	B	2006	ASP	2.8
1	B	750	LEU	2.8
1	B	438	GLN	2.8
1	B	2046	GLU	2.7
1	B	2034	PRO	2.7
1	B	1368	LEU	2.7
1	B	2042	GLU	2.7
1	B	689	TYR	2.7
1	B	2012	ASN	2.7
1	B	464	VAL	2.7
1	B	774	LEU	2.6
1	B	778	LEU	2.6
1	B	1990	ASP	2.6
1	B	472	GLN	2.6
1	B	1776	ILE	2.6
1	B	1869	ARG	2.6
1	B	1992	GLU	2.6
1	B	2094	PHE	2.6
1	B	562	TYR	2.5
1	B	709	TYR	2.5
1	B	2040	GLN	2.5
1	B	1998	GLN	2.5
1	B	1423	ASN	2.5
1	B	2029	ILE	2.5
1	B	2099	THR	2.5
1	B	787	ALA	2.5
1	B	529	GLY	2.5
1	B	2068	ILE	2.5
1	B	444	GLU	2.5
1	B	1936	LEU	2.5
1	B	432	ASP	2.5
1	B	2103	ASN	2.4
1	B	575	LEU	2.4
1	B	1908	LEU	2.4
1	B	1321	TYR	2.4
1	B	746	ASP	2.4
1	B	1956	LYS	2.4
1	B	2055	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	2076	LEU	2.4
1	B	753	ARG	2.4
1	B	1170	MET	2.3
1	B	1970	HIS	2.3
1	B	475	PHE	2.3
1	B	2107	TYR	2.3
1	B	2123	SER	2.3
1	B	2023	VAL	2.3
1	B	738	ILE	2.3
1	B	772	LEU	2.3
1	B	2021	TYR	2.3
1	B	468	PRO	2.3
1	B	2025	ASP	2.2
1	B	462	LEU	2.2
1	B	875	GLU	2.2
1	B	1315	SER	2.2
1	B	2089	LYS	2.2
1	B	784	ILE	2.2
1	B	1994	ASN	2.2
1	B	445	VAL	2.2
1	B	2028	SER	2.1
1	B	1893	LEU	2.1
1	B	1135	LEU	2.1
1	B	601	GLY	2.1
1	B	1878	LYS	2.1
1	B	2032	GLY	2.1
1	B	2116	CYS	2.1
1	B	1035	LEU	2.1
1	B	1145	LYS	2.1
1	B	2101	ALA	2.1
1	B	1984	ASP	2.0
1	B	441	GLY	2.0
1	B	870	ILE	2.0
1	B	599	LYS	2.0
1	B	1773	LEU	2.0
1	B	2030	ARG	2.0
1	B	1870	GLN	2.0
1	B	2072	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ADP	B	3001	27/27	0.90	0.24	0.56	116,145,168,183	0
5	SAN	B	3004	11/11	0.95	0.20	0.05	96,102,121,132	0
3	ATP	B	3002	31/31	0.93	0.20	-0.09	87,120,199,217	0
4	MG	B	3003	1/1	0.89	0.56	-	164,164,164,164	0

6.5 Other polymers [i](#)

There are no such residues in this entry.