



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:38 pm BST

PDB ID : 4KIT
Title : Crystal structure of human Brr2 in complex with the Prp8 Jab1/MPN domain
Authors : Wahl, M.C.; Wandersleben, T.; Santos, K.F.
Deposited on : 2013-05-02
Resolution : 3.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

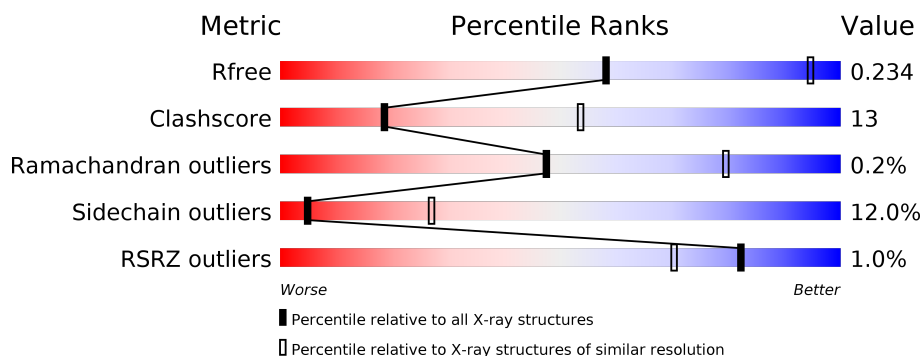
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 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	1739	<div> <div></div> <div>64%</div> <div>30%</div> <div>5%</div> </div>
2	C	278	<div> <div></div> <div>60%</div> <div>32%</div> <div></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	B	2201	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16086 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	1722	Total	C	N	O	S	0	0	0
			13846	8848	2369	2557	72			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	391	GLY	-	EXPRESSION TAG	UNP O75643
B	392	ALA	-	EXPRESSION TAG	UNP O75643
B	393	GLU	-	EXPRESSION TAG	UNP O75643
B	394	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	C	269	Total	C	N	O	S	0	0	0
			2185	1396	374	404	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2058	GLY	-	EXPRESSION TAG	UNP Q6P2Q9
C	2059	PRO	-	EXPRESSION TAG	UNP Q6P2Q9
C	2060	LEU	-	EXPRESSION TAG	UNP Q6P2Q9
C	2061	GLY	-	EXPRESSION TAG	UNP Q6P2Q9
C	2062	SER	-	EXPRESSION TAG	UNP Q6P2Q9
C	2063	MET	-	EXPRESSION TAG	UNP Q6P2Q9

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

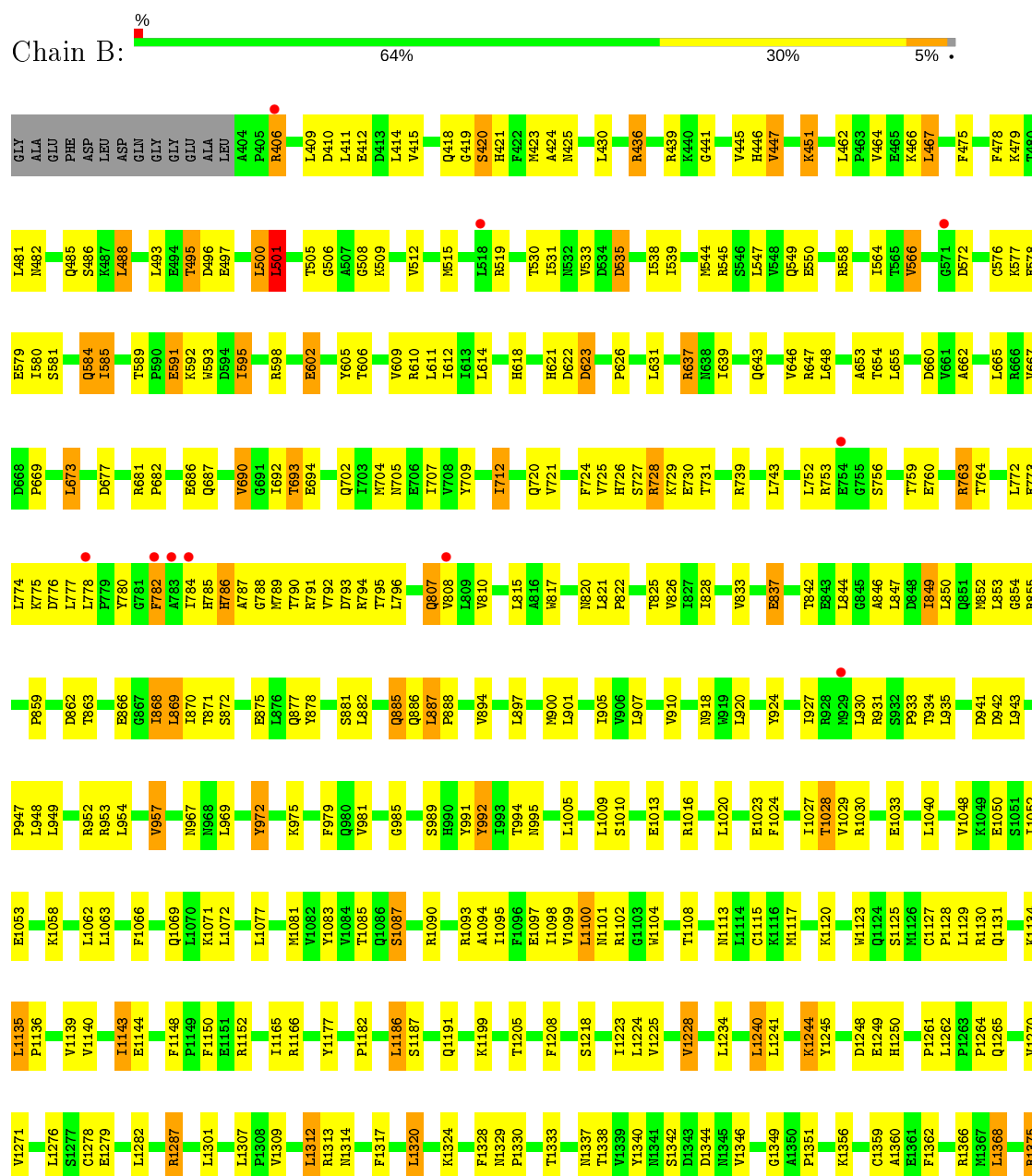
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

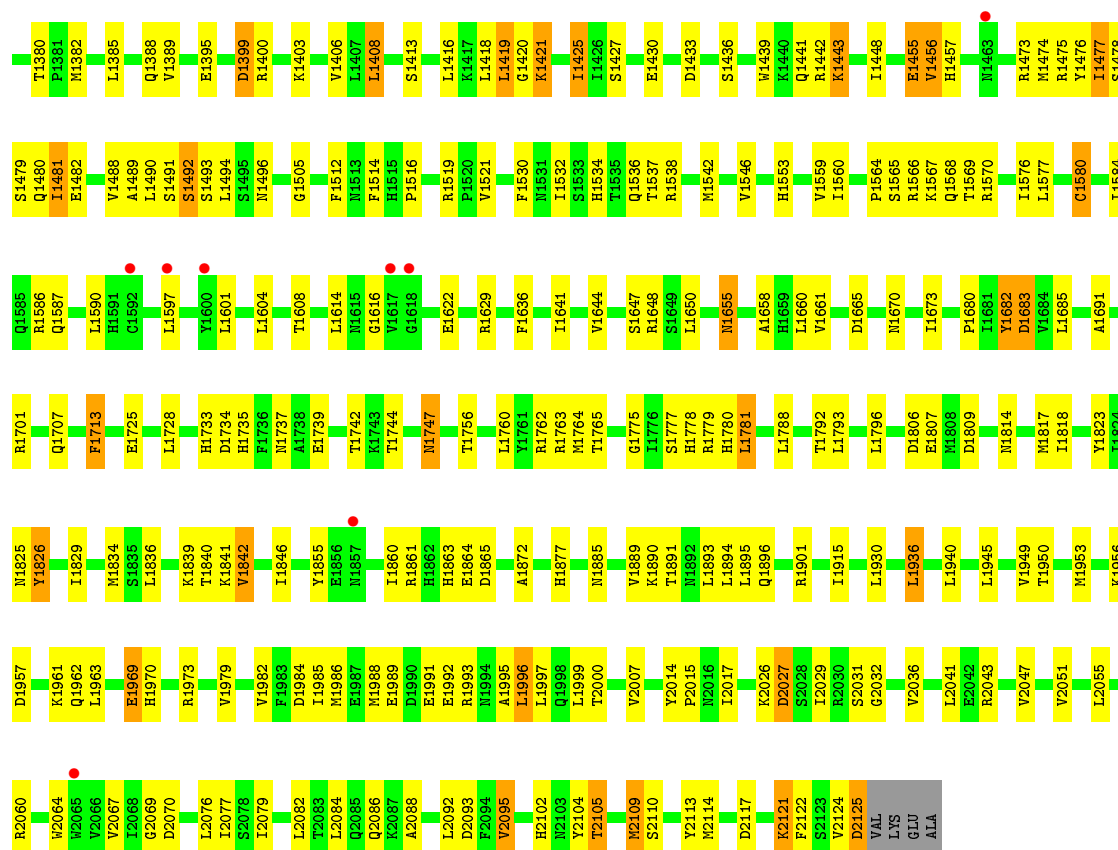
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

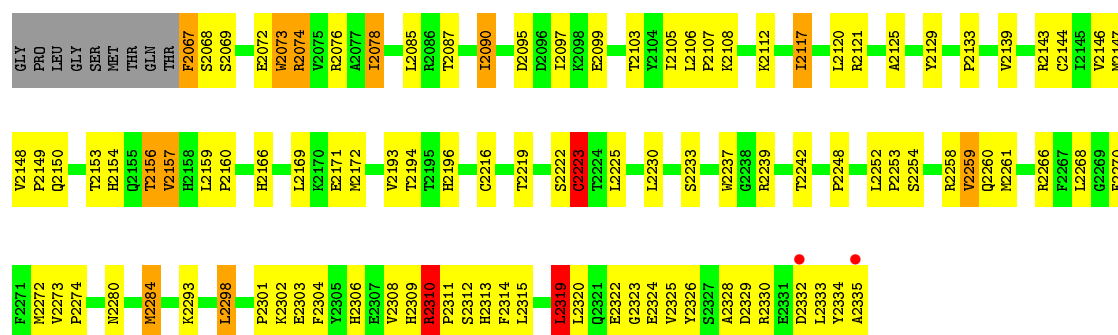
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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





• Molecule 2: Pre-mRNA-processing-splicing factor 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	240.00Å 240.00Å 201.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 3.60 49.20 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.20-3.60) 99.8 (49.20-3.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.197 , 0.235 0.197 , 0.234	Depositor DCC
R_{free} test set	3414 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	108.2	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 93.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16086	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: MG, ADP

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	0.36	0/14140	0.58	2/19159 (0.0%)
2	C	0.58	1/2253 (0.0%)	0.71	2/3066 (0.1%)
All	All	0.40	1/16393 (0.0%)	0.60	4/22225 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2223	CYS	CB-SG	-6.71	1.70	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1276	LEU	CA-CB-CG	6.14	129.43	115.30
2	C	2310	ARG	CG-CD-NE	5.39	123.11	111.80
1	B	501	LEU	CA-CB-CG	5.25	127.39	115.30
2	C	2319	LEU	CB-CG-CD2	5.02	119.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	430	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	13846	0	13985	355	0
2	C	2185	0	2106	85	0
3	B	54	0	24	3	0
4	B	1	0	0	0	0
All	All	16086	0	16115	425	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 13.

All (425) 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:1538:ARG:NH1	1:B:1665:ASP:OD1	2.10	0.84
1:B:782:PHE:HB3	1:B:808:VAL:HB	1.60	0.84
1:B:1218:SER:HB3	1:B:1240:LEU:HD21	1.61	0.82
1:B:425:ASN:ND2	1:B:886:GLN:O	2.13	0.82
1:B:591:GLU:HG3	2:C:2333:LEU:HB3	1.61	0.82
1:B:1380:THR:HG21	1:B:1385:LEU:HB3	1.65	0.79
1:B:593:TRP:HD1	1:B:631:LEU:HD22	1.46	0.78
1:B:539:ILE:HB	1:B:612:ILE:HG22	1.65	0.77
1:B:790:THR:HG21	1:B:793:ASP:HB2	1.64	0.77
1:B:424:ALA:HB3	1:B:888:PRO:HG2	1.66	0.75
1:B:686:GLU:HB2	1:B:866:GLU:HG2	1.69	0.75
2:C:2073:TRP:CD1	2:C:2074:ARG:HD2	2.22	0.73
1:B:1205:THR:HG22	1:B:1249:GLU:HB3	1.68	0.73
1:B:1739:GLU:HG3	1:B:1744:THR:HB	1.71	0.73
1:B:509:LYS:NZ	3:B:2201:ADP:O1A	2.16	0.73
1:B:731:THR:HG22	1:B:784:ILE:HB	1.71	0.73
1:B:1901:ARG:HH11	1:B:1961:LYS:HE2	1.54	0.72
2:C:2324:GLU:HG2	2:C:2330:ARG:HH12	1.54	0.72
2:C:2156:THR:OG1	2:C:2157:VAL:N	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:THR:O	1:B:794:ARG:NH1	2.25	0.70
1:B:2041:LEU:HB2	1:B:2088:ALA:HB3	1.74	0.69
1:B:1737:ASN:HB2	1:B:1796:LEU:HD21	1.73	0.69
2:C:2146:VAL:HG22	2:C:2272:MET:HB2	1.74	0.68
1:B:728:ARG:NE	2:C:2328:ALA:HB3	2.09	0.68
1:B:637:ARG:NH1	1:B:918:ASN:OD1	2.26	0.68
1:B:1963:LEU:HD22	1:B:2007:VAL:HG13	1.76	0.68
1:B:2043:ARG:HB3	1:B:2086:GLN:HA	1.76	0.68
1:B:739:ARG:NH2	1:B:776:ASP:OD2	2.27	0.67
2:C:2306:HIS:CD2	2:C:2308:VAL:H	2.13	0.67
1:B:1565:SER:HB3	1:B:1568:GLN:HB2	1.77	0.66
1:B:947:PRO:HG2	1:B:948:LEU:HD12	1.78	0.66
1:B:1338:THR:O	1:B:1342:SER:OG	2.12	0.66
1:B:1052:ILE:HG12	1:B:1053:GLU:H	1.61	0.66
1:B:1130:ARG:NH1	1:B:1144:GLU:OE1	2.29	0.66
1:B:1433:ASP:OD2	1:B:1473:ARG:NH2	2.29	0.66
1:B:1590:LEU:HD11	1:B:1597:LEU:HD11	1.78	0.65
2:C:2319:LEU:HG	2:C:2320:LEU:N	2.11	0.65
1:B:1765:THR:HG23	1:B:1781:LEU:HD13	1.79	0.65
1:B:589:THR:H	1:B:592:LYS:HE2	1.62	0.65
1:B:1456:VAL:HG11	1:B:1489:ALA:HB1	1.79	0.64
1:B:1973:ARG:HD2	1:B:1997:LEU:HD11	1.80	0.64
1:B:1950:THR:OG1	1:B:2060:ARG:NH2	2.30	0.64
1:B:1104:TRP:O	1:B:1108:THR:HG23	1.97	0.64
1:B:728:ARG:NH2	1:B:787:ALA:H	1.96	0.64
1:B:447:VAL:HG22	1:B:687:GLN:HB2	1.80	0.63
1:B:1992:GLU:HA	1:B:1995:ALA:HB3	1.80	0.63
1:B:538:ILE:HB	1:B:585:ILE:HG12	1.79	0.63
1:B:772:LEU:HB2	1:B:774:LEU:HG	1.81	0.63
1:B:508:GLY:HA3	3:B:2201:ADP:H8	1.64	0.62
2:C:2068:SER:HB2	2:C:2072:GLU:HB2	1.81	0.62
2:C:2105:ILE:HD13	2:C:2266:ARG:HH22	1.64	0.62
1:B:1553:HIS:HB3	1:B:1701:ARG:HD2	1.79	0.62
1:B:1936:LEU:HD22	1:B:1940:LEU:HD11	1.81	0.62
1:B:2067:VAL:HG22	1:B:2079:ILE:HG13	1.81	0.61
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.83	0.61
1:B:2124:VAL:O	1:B:2125:ASP:HB2	2.01	0.61
1:B:451:LYS:H	1:B:451:LYS:HE2	1.66	0.60
2:C:2129:TYR:HB3	2:C:2172:MET:HE3	1.82	0.60
1:B:1135:LEU:HD22	1:B:1140:VAL:HG23	1.84	0.60
2:C:2073:TRP:CZ3	2:C:2310:ARG:HG2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1777:SER:OG	1:B:1778:HIS:N	2.34	0.60
1:B:704:MET:HG3	1:B:870:ILE:HG21	1.83	0.60
2:C:2106:LEU:HD12	2:C:2107:PRO:HD2	1.83	0.59
1:B:844:LEU:HD11	1:B:849:ILE:HG23	1.83	0.59
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.85	0.59
1:B:728:ARG:HH21	1:B:787:ALA:H	1.50	0.59
1:B:1028:THR:O	1:B:1058:LYS:NZ	2.31	0.59
1:B:1586:ARG:HG2	1:B:1587:GLN:HG3	1.86	0.58
2:C:2073:TRP:CD1	2:C:2074:ARG:N	2.72	0.58
1:B:545:ARG:O	1:B:549:GLN:HG2	2.03	0.58
2:C:2310:ARG:NH1	2:C:2314:PHE:HE1	2.02	0.58
1:B:887:LEU:HD23	1:B:888:PRO:HD2	1.86	0.58
1:B:1307:LEU:H	1:B:1333:THR:HG21	1.69	0.58
1:B:2014:TYR:OH	1:B:2114:MET:O	2.23	0.57
1:B:764:THR:OG1	1:B:778:LEU:O	2.18	0.57
1:B:1570:ARG:NH2	1:B:1608:THR:HG21	2.18	0.57
1:B:1040:LEU:HD11	1:B:1072:LEU:HD22	1.86	0.57
1:B:1861:ARG:HD2	1:B:1864:GLU:OE2	2.05	0.57
1:B:482:ASN:HB3	1:B:485:GLN:CD	2.25	0.57
1:B:681:ARG:HH21	1:B:854:GLY:HA2	1.69	0.57
1:B:1661:VAL:HG23	1:B:1691:ALA:HB2	1.86	0.57
1:B:1670:ASN:ND2	1:B:1673:ILE:HG12	2.20	0.57
1:B:1120:LYS:HG2	1:B:1131:GLN:HG2	1.86	0.56
1:B:1989:GLU:HG2	1:B:1991:GLU:H	1.70	0.56
1:B:1985:ILE:O	1:B:1993:ARG:NH1	2.39	0.56
2:C:2073:TRP:HD1	2:C:2074:ARG:HD2	1.68	0.56
2:C:2320:LEU:HD23	2:C:2322:GLU:H	1.71	0.56
1:B:1564:PRO:O	1:B:1648:ARG:NH2	2.40	0.55
1:B:1777:SER:HB3	1:B:1780:HIS:ND1	2.21	0.55
1:B:871:THR:OG1	1:B:872:SER:N	2.39	0.55
2:C:2153:THR:HG22	2:C:2154:HIS:H	1.70	0.55
1:B:1877:HIS:HB2	1:B:1896:GLN:NE2	2.21	0.55
1:B:690:VAL:HG21	1:B:707:ILE:HD13	1.87	0.55
1:B:727:SER:HB3	1:B:730:GLU:HB3	1.89	0.55
1:B:927:ILE:HB	1:B:931:ARG:HH21	1.71	0.55
2:C:2095:ASP:OD2	2:C:2258:ARG:NE	2.36	0.55
1:B:1223:ILE:HG22	1:B:1270:VAL:HG22	1.87	0.55
2:C:2073:TRP:HD1	2:C:2074:ARG:N	2.04	0.55
1:B:1048:VAL:O	1:B:1050:GLU:N	2.40	0.55
1:B:828:ILE:HD12	1:B:869:LEU:HD12	1.87	0.55
1:B:602:GLU:HG2	1:B:606:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2306:HIS:HD2	2:C:2308:VAL:H	1.55	0.54
1:B:1005:LEU:HD11	1:B:1095:ILE:HG23	1.90	0.54
1:B:1134:LYS:HE2	1:B:1177:TYR:CE1	2.43	0.54
1:B:788:GLY:HA3	2:C:2325:VAL:HG13	1.89	0.54
1:B:2069:GLY:HA2	1:B:2077:ILE:HB	1.89	0.54
1:B:752:LEU:O	1:B:807:GLN:NE2	2.40	0.54
1:B:729:LYS:HD3	2:C:2326:TYR:CE2	2.43	0.54
1:B:793:ASP:HA	1:B:796:LEU:HB2	1.89	0.54
2:C:2310:ARG:HH12	2:C:2314:PHE:HE1	1.56	0.54
1:B:991:TYR:O	1:B:1090:ARG:HD2	2.07	0.53
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.47	0.53
1:B:2105:THR:HG23	1:B:2121:LYS:HG3	1.90	0.53
1:B:785:HIS:CE1	1:B:815:LEU:HD23	2.43	0.53
1:B:1071:LYS:HB2	2:C:2323:GLY:HA3	1.90	0.53
1:B:606:THR:HA	1:B:609:VAL:HG22	1.90	0.53
1:B:791:ARG:HH21	1:B:794:ARG:HH12	1.55	0.53
2:C:2073:TRP:CH2	2:C:2310:ARG:HG2	2.44	0.53
1:B:1134:LYS:HE2	1:B:1177:TYR:HE1	1.74	0.53
1:B:1375:ARG:CZ	1:B:1420:GLY:HA2	2.39	0.53
1:B:1287:ARG:NH1	2:C:2298:LEU:HD11	2.24	0.53
2:C:2067:PHE:CE1	2:C:2069:SER:HA	2.43	0.53
1:B:425:ASN:ND2	1:B:888:PRO:HD3	2.23	0.53
1:B:593:TRP:CD1	1:B:631:LEU:HD22	2.37	0.53
2:C:2095:ASP:OD1	2:C:2095:ASP:N	2.41	0.53
1:B:2026:LYS:NZ	1:B:2027:ASP:OD2	2.42	0.52
2:C:2117:ILE:O	2:C:2304:PHE:HB2	2.07	0.52
1:B:930:LEU:HD23	1:B:949:LEU:HD23	1.92	0.52
1:B:1099:VAL:HG13	1:B:1108:THR:HG22	1.91	0.52
1:B:1601:LEU:HD23	1:B:1604:LEU:HD12	1.91	0.52
1:B:1842:VAL:O	1:B:1846:ILE:HG12	2.08	0.52
2:C:2133:PRO:HD2	2:C:2139:VAL:HG13	1.92	0.52
1:B:1380:THR:HG22	1:B:1382:MET:H	1.74	0.52
1:B:1443:LYS:H	1:B:1443:LYS:HD3	1.73	0.52
1:B:1228:VAL:CG1	1:B:1264:PRO:HD2	2.40	0.51
1:B:792:VAL:HG12	1:B:796:LEU:HD13	1.92	0.51
1:B:544:MET:HG3	1:B:817:TRP:CE2	2.46	0.51
1:B:1182:PRO:HA	1:B:1208:PHE:CG	2.45	0.51
1:B:1271:VAL:HG12	1:B:1279:GLU:HB2	1.92	0.51
1:B:1081:MET:O	1:B:1085:THR:HG23	2.11	0.51
1:B:1127:CYS:SG	1:B:1129:LEU:HB2	2.51	0.51
1:B:2064:TRP:CZ3	1:B:2110:SER:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1636:PHE:CE1	1:B:1644:VAL:HG22	2.45	0.51
1:B:1519:ARG:NH1	1:B:1521:VAL:O	2.44	0.51
1:B:1418:LEU:O	1:B:1421:LYS:HG2	2.11	0.51
2:C:2090:ILE:HA	2:C:2223:CYS:O	2.10	0.51
2:C:2147:MET:O	2:C:2274:PRO:HD3	2.10	0.51
1:B:406:ARG:HG2	1:B:954:LEU:HG	1.93	0.50
1:B:1478:SER:HA	1:B:1481:ILE:HG22	1.93	0.50
1:B:1872:ALA:HB2	1:B:1893:LEU:HD13	1.93	0.50
1:B:1891:THR:O	1:B:1895:LEU:HB2	2.11	0.50
1:B:424:ALA:HB1	1:B:935:LEU:HD11	1.93	0.50
1:B:788:GLY:O	2:C:2325:VAL:HG22	2.12	0.50
1:B:1329:ASN:O	1:B:1333:THR:HG23	2.12	0.50
1:B:1979:VAL:HG11	1:B:1985:ILE:HG23	1.92	0.50
1:B:1135:LEU:HD23	1:B:1136:PRO:HD2	1.93	0.50
1:B:1496:ASN:HD22	1:B:1763:ARG:NH1	2.09	0.50
1:B:833:VAL:CG1	1:B:844:LEU:HB3	2.42	0.50
2:C:2073:TRP:HH2	2:C:2310:ARG:NH1	2.09	0.50
1:B:1534:HIS:CE1	1:B:1536:GLN:HB2	2.47	0.50
1:B:1982:VAL:O	1:B:1986:MET:HG2	2.11	0.50
2:C:2073:TRP:CH2	2:C:2310:ARG:NH1	2.80	0.50
1:B:1100:LEU:HA	1:B:1108:THR:HG21	1.94	0.50
1:B:1890:LYS:NZ	1:B:1894:LEU:HD11	2.26	0.49
1:B:495:THR:HG22	1:B:497:GLU:H	1.77	0.49
1:B:725:VAL:HG12	1:B:727:SER:H	1.77	0.49
1:B:1512:PHE:HB3	1:B:1514:PHE:CE2	2.47	0.49
1:B:1962:GLN:HE22	1:B:2014:TYR:HE1	1.61	0.49
1:B:420:SER:HA	1:B:621:HIS:CD2	2.47	0.49
1:B:837:GLU:HG2	1:B:1083:TYR:CZ	2.48	0.49
1:B:1839:LYS:O	1:B:1841:LYS:HE3	2.13	0.49
1:B:1476:TYR:O	1:B:1479:SER:HB3	2.13	0.49
1:B:1566:ARG:O	1:B:1569:THR:HG22	2.13	0.49
1:B:441:GLY:O	1:B:693:THR:N	2.36	0.49
1:B:772:LEU:HD23	1:B:789:MET:HB2	1.95	0.49
1:B:1309:VAL:HA	1:B:1328:PHE:HE2	1.77	0.49
2:C:2149:PRO:O	2:C:2160:PRO:HD3	2.13	0.49
1:B:1725:GLU:OE1	1:B:1763:ARG:NE	2.46	0.48
1:B:787:ALA:HA	1:B:794:ARG:HD3	1.94	0.48
2:C:2097:ILE:HD12	2:C:2099:GLU:HB2	1.94	0.48
1:B:1265:GLN:HG2	1:B:1265:GLN:O	2.13	0.48
1:B:1356:LYS:O	1:B:1359:CYS:HB2	2.14	0.48
1:B:1359:CYS:HA	1:B:1362:PHE:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:LEU:HD23	1:B:662:ALA:HA	1.95	0.48
1:B:1113:ASN:O	1:B:1117:MET:HG3	2.13	0.48
1:B:512:VAL:HA	1:B:515:MET:HE2	1.95	0.48
1:B:493:LEU:HD11	1:B:515:MET:HB3	1.96	0.48
1:B:1713:PHE:N	1:B:1713:PHE:CD1	2.82	0.48
1:B:2076:LEU:HD21	1:B:2079:ILE:HB	1.96	0.48
1:B:1747:ASN:HB2	1:B:1809:ASP:HA	1.95	0.48
1:B:994:THR:HG22	1:B:1023:GLU:OE1	2.14	0.47
1:B:1616:GLY:HA2	1:B:1641:ILE:HG22	1.95	0.47
1:B:720:GLN:HG2	1:B:807:GLN:HA	1.96	0.47
1:B:1024:PHE:HB3	1:B:1027:ILE:HD12	1.96	0.47
1:B:1264:PRO:HB2	1:B:1265:GLN:OE1	2.15	0.47
1:B:1559:VAL:HG22	1:B:1660:LEU:HB3	1.95	0.47
1:B:2104:TYR:HB2	1:B:2122:PHE:CZ	2.50	0.47
1:B:420:SER:HB3	1:B:622:ASP:HA	1.97	0.47
1:B:972:TYR:HB2	1:B:979:PHE:HD1	1.79	0.47
1:B:1139:VAL:O	1:B:1143:ILE:HG23	2.13	0.47
1:B:538:ILE:HG12	1:B:611:LEU:HB3	1.96	0.47
2:C:2310:ARG:HH11	2:C:2310:ARG:CG	2.27	0.47
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.49	0.47
1:B:1375:ARG:HG2	1:B:1448:ILE:HG22	1.97	0.47
1:B:724:PHE:CG	1:B:852:MET:HE2	2.49	0.47
1:B:1408:LEU:HD23	1:B:1427:SER:HB2	1.95	0.47
1:B:828:ILE:HD13	1:B:849:ILE:HG22	1.96	0.47
1:B:1408:LEU:HD22	1:B:1425:ILE:HG22	1.95	0.47
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.96	0.47
1:B:1796:LEU:HA	1:B:1796:LEU:HD12	1.70	0.47
1:B:1969:GLU:H	1:B:1969:GLU:HG3	1.59	0.47
1:B:772:LEU:H	1:B:772:LEU:HD12	1.80	0.47
1:B:969:LEU:CD1	1:B:985:GLY:HA2	2.45	0.46
1:B:530:THR:C	1:B:531:ILE:HG13	2.36	0.46
1:B:618:HIS:CD2	1:B:847:LEU:HD22	2.49	0.46
2:C:2148:VAL:O	2:C:2150:GLN:HG2	2.14	0.46
2:C:2252:LEU:HD23	2:C:2253:PRO:HD2	1.96	0.46
1:B:1228:VAL:HG11	1:B:1264:PRO:HD2	1.97	0.46
1:B:1320:LEU:HA	1:B:1400:ARG:NH1	2.30	0.46
1:B:1982:VAL:HG13	1:B:1985:ILE:HD11	1.95	0.46
1:B:967:ASN:ND2	1:B:995:ASN:O	2.48	0.46
1:B:1329:ASN:HB2	1:B:1330:PRO:HD2	1.98	0.46
1:B:969:LEU:HD12	1:B:985:GLY:HA2	1.96	0.46
2:C:2196:HIS:HB3	2:C:2230:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2272:MET:HE3	2:C:2272:MET:HB3	1.65	0.46
2:C:2121:ARG:O	2:C:2154:HIS:HA	2.15	0.46
1:B:1532:ILE:HG21	1:B:1537:THR:HB	1.97	0.46
1:B:418:GLN:HE22	1:B:842:THR:HG22	1.81	0.46
1:B:1775:GLY:HA3	1:B:1780:HIS:CD2	2.51	0.46
1:B:791:ARG:HH21	1:B:794:ARG:NH1	2.13	0.46
2:C:2303:GLU:H	2:C:2303:GLU:CD	2.19	0.46
1:B:669:PRO:HA	1:B:673:LEU:HB2	1.97	0.46
1:B:728:ARG:HD2	1:B:728:ARG:HA	1.59	0.46
1:B:1028:THR:OG1	1:B:1029:VAL:N	2.49	0.45
1:B:1328:PHE:HB2	1:B:1333:THR:HG22	1.97	0.45
1:B:1349:GLY:HA2	1:B:1491:SER:O	2.16	0.45
1:B:1760:LEU:O	1:B:1764:MET:HG3	2.15	0.45
1:B:1314:ASN:OD1	1:B:1317:PHE:N	2.47	0.45
2:C:2074:ARG:O	2:C:2078:ILE:HD13	2.17	0.45
1:B:1889:VAL:O	1:B:1893:LEU:HG	2.17	0.45
1:B:1324:LYS:NZ	1:B:1400:ARG:HH12	2.14	0.45
1:B:1395:GLU:HA	1:B:1399:ASP:HB2	1.98	0.45
1:B:531:ILE:HD12	1:B:531:ILE:O	2.16	0.45
1:B:791:ARG:HE	1:B:794:ARG:HH22	1.64	0.45
1:B:420:SER:O	1:B:878:TYR:OH	2.26	0.45
1:B:421:HIS:NE2	1:B:875:GLU:OE1	2.49	0.45
1:B:506:GLY:O	1:B:682:PRO:HG3	2.15	0.45
1:B:881:SER:HA	1:B:886:GLN:HB2	1.99	0.45
1:B:1439:TRP:CD2	1:B:1477:ILE:HD13	2.52	0.45
1:B:1534:HIS:HE1	1:B:1536:GLN:HB2	1.81	0.45
1:B:1733:HIS:CD2	1:B:1792:THR:HG23	2.52	0.45
1:B:665:LEU:HB2	1:B:667:VAL:HG23	1.99	0.45
1:B:728:ARG:NH2	1:B:786:HIS:HB2	2.31	0.45
1:B:833:VAL:HG11	1:B:844:LEU:HB3	1.98	0.45
2:C:2237:TRP:HZ2	2:C:2248:PRO:HB2	1.82	0.45
1:B:509:LYS:HE2	1:B:509:LYS:HB2	1.66	0.45
1:B:826:VAL:O	1:B:868:ILE:HD12	2.16	0.45
2:C:2073:TRP:CZ3	2:C:2313:HIS:CE1	3.05	0.45
1:B:592:LYS:HG3	2:C:2335:ALA:H	1.82	0.45
1:B:544:MET:HG3	1:B:817:TRP:CD2	2.53	0.44
1:B:1359:CYS:HA	1:B:1362:PHE:HD2	1.82	0.44
1:B:728:ARG:HH21	1:B:787:ALA:N	2.13	0.44
2:C:2169:LEU:HD21	2:C:2272:MET:HG3	1.98	0.44
1:B:1191:GLN:HE21	1:B:1199:LYS:HE2	1.82	0.44
1:B:1735:HIS:O	1:B:1739:GLU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2073:TRP:C	2:C:2073:TRP:CD1	2.91	0.44
1:B:1123:TRP:CG	2:C:2314:PHE:HD2	2.36	0.44
1:B:1475:ARG:HH12	1:B:1505:GLY:HA3	1.82	0.44
1:B:1475:ARG:NH1	1:B:1505:GLY:HA3	2.32	0.44
1:B:1530:PHE:CD2	1:B:1542:MET:HE2	2.53	0.44
1:B:846:ALA:O	1:B:849:ILE:HG13	2.16	0.44
1:B:598:ARG:HA	1:B:907:LEU:HD21	1.98	0.44
1:B:721:VAL:HA	1:B:825:THR:O	2.17	0.44
1:B:822:PRO:HG2	1:B:859:PRO:HD3	1.99	0.44
1:B:412:GLU:O	1:B:415:VAL:HG22	2.17	0.44
2:C:2222:SER:OG	2:C:2223:CYS:N	2.50	0.44
1:B:1340:TYR:O	1:B:1366:ARG:HD2	2.18	0.44
2:C:2121:ARG:HA	2:C:2121:ARG:HD2	1.55	0.44
2:C:2280:ASN:HB3	2:C:2309:HIS:CD2	2.52	0.44
1:B:1010:SER:OG	1:B:1013:GLU:OE2	2.33	0.44
1:B:828:ILE:HD11	1:B:853:LEU:HD13	2.00	0.44
2:C:2073:TRP:CH2	2:C:2313:HIS:CG	3.06	0.44
1:B:1457:HIS:CE1	1:B:1492:SER:HB3	2.53	0.43
1:B:1945:LEU:O	1:B:1949:VAL:HG23	2.18	0.43
1:B:2032:GLY:HA2	1:B:2095:VAL:HG23	2.00	0.43
1:B:496:ASP:CG	1:B:519:ARG:HH11	2.22	0.43
1:B:1128:PRO:HG2	1:B:1150:PHE:CD2	2.52	0.43
1:B:462:LEU:HD21	1:B:467:LEU:HB3	2.01	0.43
1:B:1094:ALA:O	1:B:1098:ILE:HG13	2.18	0.43
1:B:1346:VAL:HG23	1:B:1488:VAL:HG13	2.01	0.43
1:B:1368:LEU:HD11	1:B:1403:LYS:HG3	2.00	0.43
1:B:592:LYS:HA	1:B:595:ILE:HD11	2.00	0.43
1:B:612:ILE:HD11	1:B:648:LEU:HG	1.98	0.43
1:B:692:ILE:HG22	1:B:694:GLU:H	1.83	0.43
2:C:2302:LYS:HD2	2:C:2306:HIS:CE1	2.53	0.43
1:B:837:GLU:HG2	1:B:1083:TYR:CE2	2.54	0.43
1:B:1344:ASP:OD2	1:B:1344:ASP:N	2.48	0.43
1:B:1455:GLU:HG3	1:B:1457:HIS:CE1	2.53	0.43
1:B:1855:TYR:CE1	1:B:1915:ILE:HG23	2.54	0.43
1:B:462:LEU:HD11	1:B:466:LYS:HB2	2.01	0.43
1:B:1033:GLU:HB3	1:B:1077:LEU:HD11	2.01	0.43
1:B:1416:LEU:O	1:B:1419:LEU:HD23	2.18	0.43
1:B:1542:MET:O	1:B:1546:VAL:HG23	2.19	0.43
1:B:464:VAL:HG21	1:B:478:PHE:O	2.18	0.43
1:B:1123:TRP:HB3	2:C:2314:PHE:HD2	1.83	0.43
1:B:2109:MET:HG3	1:B:2117:ASP:CG	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:ASP:OD1	1:B:535:ASP:N	2.50	0.43
1:B:729:LYS:HD3	2:C:2326:TYR:HE2	1.82	0.43
2:C:2072:GLU:O	2:C:2076:ARG:HG3	2.19	0.43
1:B:1836:LEU:HB3	1:B:1930:LEU:HD21	2.01	0.43
1:B:862:ASP:OD1	1:B:863:THR:N	2.52	0.43
1:B:1244:LYS:HE2	1:B:1245:TYR:CE2	2.54	0.43
1:B:1647:SER:HB3	1:B:1650:LEU:HD13	2.01	0.42
1:B:1825:ASN:OD1	1:B:1826:TYR:N	2.52	0.42
1:B:2051:VAL:HG13	1:B:2113:TYR:CZ	2.54	0.42
1:B:623:ASP:O	1:B:626:PRO:HD2	2.19	0.42
1:B:655:LEU:HD21	1:B:882:LEU:HD23	2.01	0.42
1:B:726:HIS:CG	1:B:833:VAL:HG12	2.54	0.42
1:B:1385:LEU:O	1:B:1389:VAL:HG23	2.19	0.42
1:B:1388:GLN:HG3	1:B:1655:ASN:OD1	2.19	0.42
1:B:1680:PRO:O	1:B:1683:ASP:HB2	2.20	0.42
1:B:479:LYS:HD3	1:B:479:LYS:HA	1.92	0.42
1:B:1261:PRO:HB2	2:C:2268:LEU:HD21	2.01	0.42
1:B:991:TYR:CE1	1:B:1097:GLU:HG3	2.54	0.42
1:B:1148:PHE:CE1	1:B:1152:ARG:HB3	2.54	0.42
1:B:1313:ARG:HD2	1:B:1313:ARG:HA	1.68	0.42
1:B:1566:ARG:HG3	1:B:1622:GLU:HG2	2.00	0.42
1:B:681:ARG:NH2	1:B:854:GLY:HA2	2.34	0.42
1:B:882:LEU:HA	1:B:882:LEU:HD23	1.79	0.42
1:B:887:LEU:HA	1:B:888:PRO:HD3	1.92	0.42
1:B:1996:LEU:HD12	1:B:1997:LEU:HD23	2.00	0.42
1:B:2027:ASP:N	1:B:2027:ASP:OD1	2.49	0.42
1:B:564:ILE:HG13	1:B:584:GLN:HG3	2.01	0.42
1:B:639:ILE:HD11	1:B:646:VAL:HB	2.01	0.42
1:B:618:HIS:CE1	1:B:653:ALA:H	2.38	0.42
2:C:2125:ALA:O	2:C:2150:GLN:NE2	2.50	0.42
2:C:2310:ARG:HH11	2:C:2310:ARG:HB3	1.83	0.42
1:B:1368:LEU:HA	1:B:1368:LEU:HD13	1.87	0.42
1:B:1890:LYS:HZ2	1:B:1894:LEU:HD11	1.83	0.42
1:B:423:MET:HB2	1:B:878:TYR:HD1	1.85	0.42
1:B:598:ARG:HD3	1:B:989:SER:OG	2.19	0.42
1:B:709:TYR:O	1:B:712:ILE:HG22	2.20	0.42
1:B:739:ARG:HD3	1:B:780:TYR:CE1	2.55	0.42
1:B:924:TYR:O	1:B:927:ILE:HG13	2.20	0.42
1:B:1009:LEU:HD23	1:B:1009:LEU:HA	1.69	0.42
1:B:2014:TYR:HA	1:B:2015:PRO:HD3	1.87	0.42
1:B:411:LEU:O	1:B:415:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2067:PHE:HB2	2:C:2072:GLU:HG2	2.00	0.42
2:C:2310:ARG:HG2	2:C:2310:ARG:HH11	1.84	0.42
1:B:752:LEU:HB3	1:B:807:GLN:HE21	1.85	0.42
1:B:1814:ASN:O	1:B:1818:ILE:HG13	2.20	0.42
1:B:566:VAL:HG23	1:B:585:ILE:O	2.20	0.42
2:C:2112:LYS:HB3	2:C:2112:LYS:HE2	1.67	0.42
2:C:2284:MET:HE1	2:C:2311:PRO:HG3	2.00	0.42
1:B:1083:TYR:O	1:B:1087:SER:OG	2.35	0.42
1:B:1186:LEU:HD13	1:B:1282:LEU:HB2	2.02	0.42
1:B:1380:THR:HG21	1:B:1385:LEU:HD22	2.01	0.42
1:B:1713:PHE:N	1:B:1713:PHE:HD1	2.17	0.42
1:B:2036:VAL:HG22	1:B:2093:ASP:HB3	2.02	0.42
1:B:481:LEU:HD23	1:B:486:SER:HA	2.02	0.42
1:B:580:ILE:HB	1:B:605:TYR:OH	2.20	0.41
2:C:2120:LEU:HD12	2:C:2120:LEU:N	2.35	0.41
1:B:1077:LEU:H	1:B:1077:LEU:HD12	1.85	0.41
1:B:777:LEU:HB3	1:B:782:PHE:O	2.21	0.41
1:B:1953:MET:HB3	1:B:1953:MET:HE2	1.99	0.41
2:C:2216:CYS:HA	2:C:2225:LEU:HB3	2.01	0.41
1:B:1493:SER:OG	1:B:1514:PHE:O	2.31	0.41
1:B:598:ARG:CZ	1:B:992:TYR:CE1	3.03	0.41
1:B:646:VAL:HG12	1:B:647:ARG:O	2.19	0.41
1:B:760:GLU:HB3	1:B:763:ARG:HB2	2.01	0.41
1:B:791:ARG:HE	1:B:794:ARG:HH12	1.68	0.41
1:B:821:LEU:HA	1:B:822:PRO:HD3	1.82	0.41
1:B:1860:ILE:HG13	1:B:1885:ASN:O	2.19	0.41
1:B:2109:MET:HG3	1:B:2117:ASP:OD1	2.20	0.41
1:B:406:ARG:HD2	1:B:406:ARG:H	1.85	0.41
1:B:948:LEU:O	1:B:953:ARG:NH1	2.53	0.41
2:C:2073:TRP:CZ3	2:C:2313:HIS:CG	3.09	0.41
1:B:488:LEU:HD21	1:B:501:LEU:HD23	2.02	0.41
1:B:509:LYS:HE2	3:B:2201:ADP:O2B	2.20	0.41
1:B:753:ARG:NE	1:B:756:SER:O	2.52	0.41
2:C:2120:LEU:HD12	2:C:2120:LEU:H	1.86	0.41
1:B:728:ARG:HG2	2:C:2328:ALA:H	1.85	0.41
1:B:1261:PRO:HB2	2:C:2268:LEU:CD2	2.51	0.41
1:B:1936:LEU:HD23	1:B:1936:LEU:HA	1.79	0.41
1:B:654:THR:OG1	1:B:885:GLN:HG2	2.21	0.41
2:C:2320:LEU:HD21	2:C:2322:GLU:CD	2.41	0.41
1:B:1312:LEU:H	1:B:1312:LEU:HD12	1.85	0.41
1:B:1576:ILE:O	1:B:1580:CYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ARG:HH11	1:B:445:VAL:HG21	1.86	0.41
1:B:933:PRO:HG3	1:B:943:LEU:HD22	2.02	0.41
2:C:2315:LEU:HD13	2:C:2315:LEU:HA	1.82	0.41
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	2.01	0.41
1:B:1494:LEU:HD12	1:B:1494:LEU:HA	1.79	0.41
1:B:481:LEU:HB3	1:B:486:SER:OG	2.21	0.41
1:B:752:LEU:HB3	1:B:807:GLN:NE2	2.36	0.41
1:B:1979:VAL:HG13	1:B:1984:ASP:HB2	2.02	0.41
1:B:577:LYS:O	1:B:581:SER:N	2.54	0.41
1:B:702:GLN:O	1:B:705:ASN:HB2	2.21	0.41
1:B:792:VAL:O	1:B:795:THR:OG1	2.30	0.41
2:C:2074:ARG:HG2	2:C:2074:ARG:H	1.63	0.41
2:C:2117:ILE:HG21	2:C:2301:PRO:HB2	2.02	0.41
1:B:1590:LEU:HD22	1:B:1614:LEU:O	2.20	0.40
1:B:1793:LEU:HD23	1:B:1793:LEU:HA	1.90	0.40
1:B:436:ARG:HG3	1:B:445:VAL:HG22	2.02	0.40
2:C:2090:ILE:H	2:C:2090:ILE:HD13	1.86	0.40
1:B:1069:GLN:C	2:C:2319:LEU:HD13	2.41	0.40
1:B:991:TYR:HE1	1:B:1097:GLU:HG3	1.85	0.40
1:B:1228:VAL:H	1:B:1228:VAL:HG23	1.52	0.40
1:B:419:GLY:C	1:B:421:HIS:H	2.25	0.40
1:B:420:SER:CB	1:B:622:ASP:HA	2.52	0.40
1:B:660:ASP:HB3	1:B:927:ILE:CD1	2.52	0.40
2:C:2144:CYS:HB2	2:C:2270:PHE:CE2	2.57	0.40
2:C:2332:ASP:O	2:C:2334:TYR:N	2.54	0.40
1:B:729:LYS:HA	1:B:729:LYS:HD2	1.72	0.40
2:C:2166:HIS:CD2	2:C:2272:MET:CE	3.05	0.40
1:B:1481:ILE:O	1:B:1481:ILE:HG12	2.20	0.40
1:B:1577:LEU:HA	1:B:1577:LEU:HD23	1.88	0.40
1:B:1682:TYR:HA	1:B:1685:LEU:HD12	2.03	0.40
1:B:439:ARG:HA	1:B:439:ARG:HD2	1.87	0.40
1:B:538:ILE:O	1:B:585:ILE:HA	2.21	0.40
2:C:2259:VAL:HG22	2:C:2260:GLN:H	1.86	0.40
1:B:1806:ASP:O	1:B:1807:GLU:HB2	2.22	0.40
1:B:612:ILE:HD12	1:B:612:ILE:O	2.21	0.40
2:C:2090:ILE:N	2:C:2090:ILE:HD13	2.37	0.40
2:C:2117:ILE:HG22	2:C:2303:GLU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1720/1739 (99%)	1633 (95%)	84 (5%)	3 (0%)	47	79
2	C	267/278 (96%)	255 (96%)	12 (4%)	0	100	100
All	All	1987/2017 (98%)	1888 (95%)	96 (5%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	957	VAL
1	B	1584	ILE
1	B	585	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1541/1552 (99%)	1361 (88%)	180 (12%)	5	29
2	C	241/248 (97%)	208 (86%)	33 (14%)	3	22
All	All	1782/1800 (99%)	1569 (88%)	213 (12%)	5	27

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	406	ARG
1	B	409	LEU
1	B	410	ASP

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Mol	Chain	Res	Type
1	B	414	LEU
1	B	420	SER
1	B	436	ARG
1	B	446	HIS
1	B	447	VAL
1	B	451	LYS
1	B	467	LEU
1	B	475	PHE
1	B	488	LEU
1	B	495	THR
1	B	500	LEU
1	B	501	LEU
1	B	505	THR
1	B	533	VAL
1	B	535	ASP
1	B	547	LEU
1	B	550	GLU
1	B	558	ARG
1	B	566	VAL
1	B	572	ASP
1	B	576	CYS
1	B	578	GLU
1	B	579	GLU
1	B	584	GLN
1	B	591	GLU
1	B	595	ILE
1	B	602	GLU
1	B	610	ARG
1	B	614	LEU
1	B	623	ASP
1	B	637	ARG
1	B	643	GLN
1	B	673	LEU
1	B	677	ASP
1	B	690	VAL
1	B	693	THR
1	B	712	ILE
1	B	728	ARG
1	B	743	LEU
1	B	759	THR
1	B	763	ARG
1	B	773	GLU

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Mol	Chain	Res	Type
1	B	775	LYS
1	B	782	PHE
1	B	786	HIS
1	B	807	GLN
1	B	810	VAL
1	B	820	ASN
1	B	837	GLU
1	B	849	ILE
1	B	850	LEU
1	B	855	ARG
1	B	868	ILE
1	B	869	LEU
1	B	877	GLN
1	B	885	GLN
1	B	887	LEU
1	B	894	VAL
1	B	897	LEU
1	B	900	MET
1	B	901	LEU
1	B	910	VAL
1	B	920	LEU
1	B	934	THR
1	B	941	ASP
1	B	942	ASP
1	B	952	ARG
1	B	957	VAL
1	B	972	TYR
1	B	975	LYS
1	B	992	TYR
1	B	1016	ARG
1	B	1020	LEU
1	B	1028	THR
1	B	1030	ARG
1	B	1062	LEU
1	B	1063	LEU
1	B	1087	SER
1	B	1100	LEU
1	B	1101	ASN
1	B	1102	ARG
1	B	1125	SER
1	B	1135	LEU
1	B	1143	ILE

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Mol	Chain	Res	Type
1	B	1165	ILE
1	B	1166	ARG
1	B	1186	LEU
1	B	1187	SER
1	B	1224	LEU
1	B	1225	VAL
1	B	1228	VAL
1	B	1234	LEU
1	B	1240	LEU
1	B	1241	LEU
1	B	1244	LYS
1	B	1248	ASP
1	B	1250	HIS
1	B	1262	LEU
1	B	1278	CYS
1	B	1287	ARG
1	B	1301	LEU
1	B	1312	LEU
1	B	1320	LEU
1	B	1337	ASN
1	B	1368	LEU
1	B	1375	ARG
1	B	1399	ASP
1	B	1406	VAL
1	B	1408	LEU
1	B	1413	SER
1	B	1419	LEU
1	B	1421	LYS
1	B	1425	ILE
1	B	1430	GLU
1	B	1436	SER
1	B	1441	GLN
1	B	1442	ARG
1	B	1443	LYS
1	B	1455	GLU
1	B	1456	VAL
1	B	1474	MET
1	B	1477	ILE
1	B	1480	GLN
1	B	1481	ILE
1	B	1482	GLU
1	B	1492	SER

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Mol	Chain	Res	Type
1	B	1567	LYS
1	B	1580	CYS
1	B	1629	ARG
1	B	1655	ASN
1	B	1682	TYR
1	B	1683	ASP
1	B	1707	GLN
1	B	1713	PHE
1	B	1728	LEU
1	B	1734	ASP
1	B	1742	THR
1	B	1747	ASN
1	B	1756	THR
1	B	1762	ARG
1	B	1779	ARG
1	B	1781	LEU
1	B	1788	LEU
1	B	1817	MET
1	B	1823	TYR
1	B	1826	TYR
1	B	1829	ILE
1	B	1834	MET
1	B	1840	THR
1	B	1842	VAL
1	B	1863	HIS
1	B	1865	ASP
1	B	1936	LEU
1	B	1956	LYS
1	B	1957	ASP
1	B	1969	GLU
1	B	1970	HIS
1	B	1988	MET
1	B	1996	LEU
1	B	1999	LEU
1	B	2000	THR
1	B	2017	ILE
1	B	2027	ASP
1	B	2029	ILE
1	B	2031	SER
1	B	2047	VAL
1	B	2055	LEU
1	B	2070	ASP

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Mol	Chain	Res	Type
1	B	2082	LEU
1	B	2084	LEU
1	B	2092	LEU
1	B	2095	VAL
1	B	2102	HIS
1	B	2105	THR
1	B	2109	MET
1	B	2121	LYS
1	B	2125	ASP
2	C	2067	PHE
2	C	2073	TRP
2	C	2074	ARG
2	C	2078	ILE
2	C	2085	LEU
2	C	2087	THR
2	C	2090	ILE
2	C	2103	THR
2	C	2108	LYS
2	C	2117	ILE
2	C	2143	ARG
2	C	2156	THR
2	C	2157	VAL
2	C	2159	LEU
2	C	2171	GLU
2	C	2193	VAL
2	C	2194	THR
2	C	2219	THR
2	C	2223	CYS
2	C	2233	SER
2	C	2239	ARG
2	C	2242	THR
2	C	2254	SER
2	C	2259	VAL
2	C	2261	MET
2	C	2273	VAL
2	C	2284	MET
2	C	2293	LYS
2	C	2298	LEU
2	C	2310	ARG
2	C	2312	SER
2	C	2319	LEU
2	C	2329	ASP

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	425	ASN
2	C	2123	GLN
2	C	2306	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 3 ligands modelled in this entry, 1 is 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	ADP	B	2202	4	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)
3	ADP	B	2201	-	24,29,29	0.97	1 (4%)	29,45,45	1.34	4 (13%)

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	ADP	B	2202	4	-	2/12/32/32	0/3/3/3
3	ADP	B	2201	-	-	8/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2201	ADP	C5-C4	2.48	1.47	1.40
3	B	2202	ADP	C5-C4	2.32	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2202	ADP	PA-O3A-PB	-4.02	119.02	132.83
3	B	2201	ADP	N3-C2-N1	-3.22	123.65	128.68
3	B	2202	ADP	C3'-C2'-C1'	3.11	105.66	100.98
3	B	2202	ADP	N3-C2-N1	-2.97	124.03	128.68
3	B	2202	ADP	C4-C5-N7	-2.86	106.42	109.40
3	B	2201	ADP	C3'-C2'-C1'	2.76	105.14	100.98
3	B	2201	ADP	PA-O3A-PB	-2.45	124.42	132.83
3	B	2201	ADP	C4-C5-N7	-2.35	106.95	109.40

There are no chirality outliers.

All (10) torsion outliers are listed below:

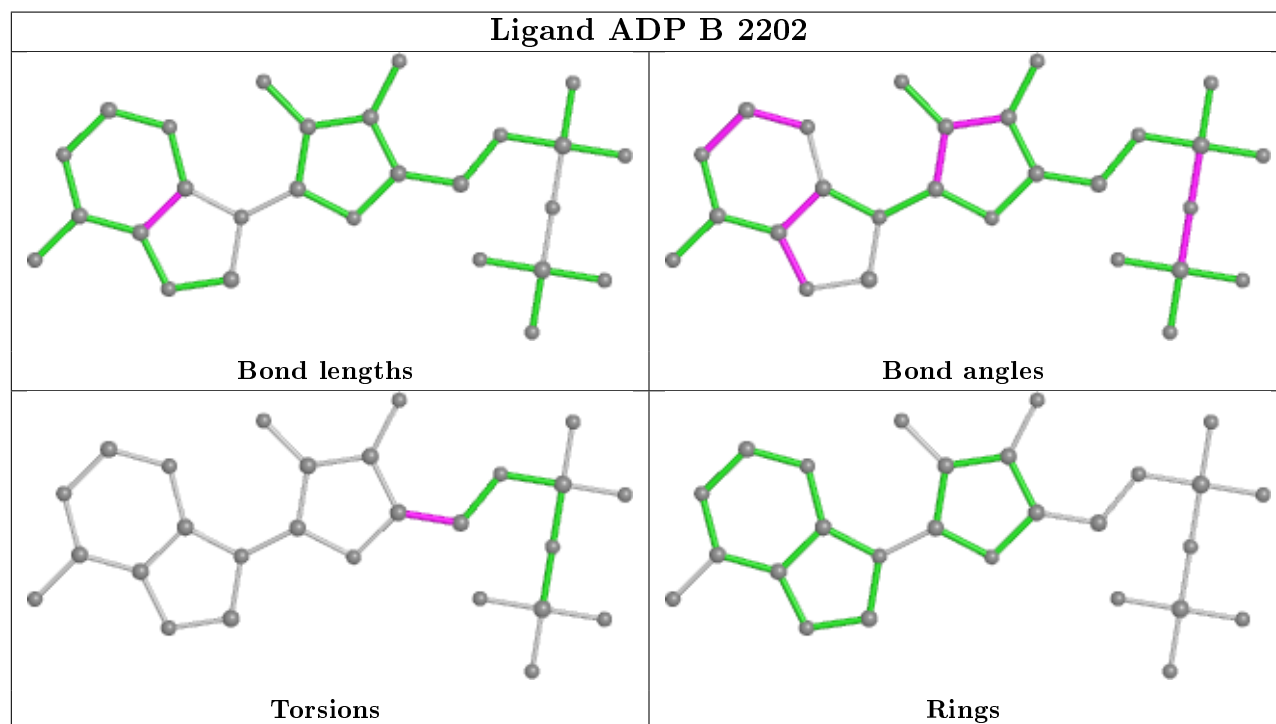
Mol	Chain	Res	Type	Atoms
3	B	2201	ADP	PA-O3A-PB-O2B
3	B	2201	ADP	C5'-O5'-PA-O1A
3	B	2201	ADP	C5'-O5'-PA-O2A
3	B	2201	ADP	C3'-C4'-C5'-O5'
3	B	2201	ADP	O4'-C4'-C5'-O5'
3	B	2202	ADP	C3'-C4'-C5'-O5'
3	B	2202	ADP	O4'-C4'-C5'-O5'
3	B	2201	ADP	PA-O3A-PB-O1B
3	B	2201	ADP	PA-O3A-PB-O3B
3	B	2201	ADP	C5'-O5'-PA-O3A

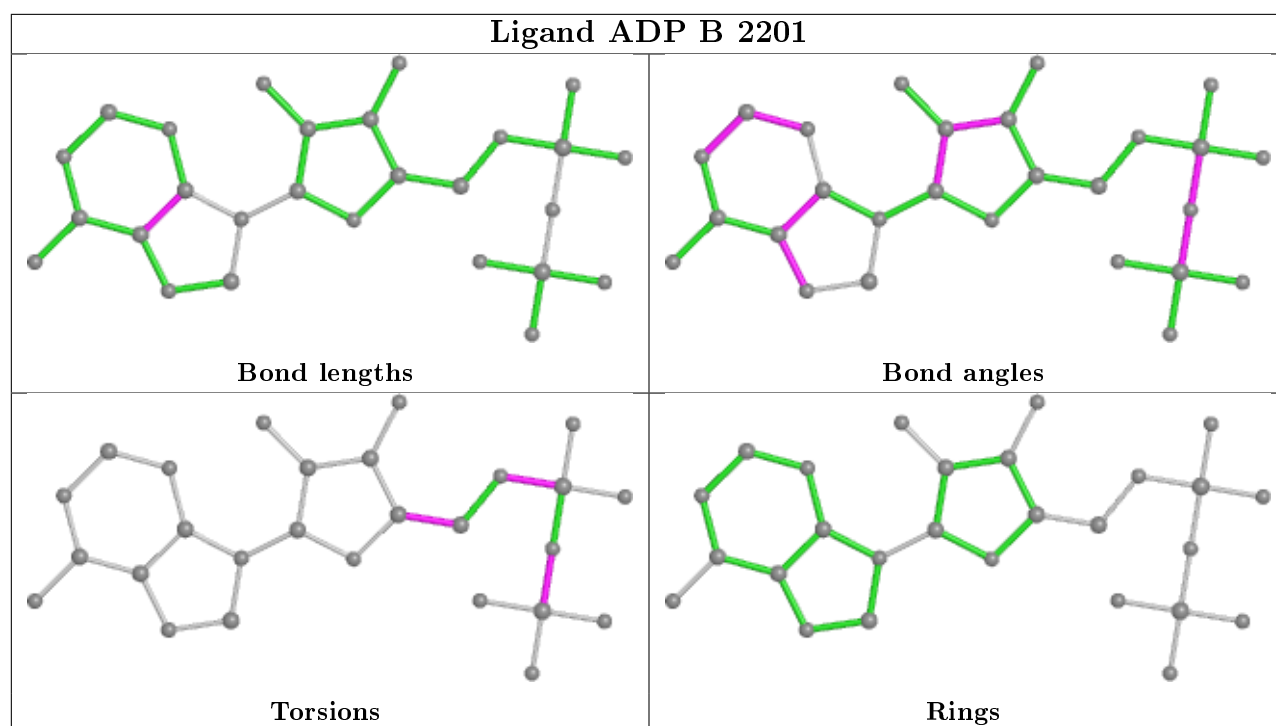
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2201	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	1722/1739 (99%)	-0.25	18 (1%) 82 70	78, 164, 238, 350	0
2	C	269/278 (96%)	-0.38	2 (0%) 87 78	65, 104, 243, 376	0
All	All	1991/2017 (98%)	-0.27	20 (1%) 82 70	65, 159, 239, 376	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	784	ILE	3.9
1	B	406	ARG	3.6
1	B	1463	ASN	3.5
1	B	783	ALA	3.4
2	C	2335	ALA	3.3
2	C	2332	ASP	3.2
1	B	1618	GLY	2.8
1	B	808	VAL	2.7
1	B	571	GLY	2.7
1	B	929	MET	2.6
1	B	1617	VAL	2.5
1	B	1597	LEU	2.4
1	B	754	GLU	2.4
1	B	1592	CYS	2.3
1	B	778	LEU	2.3
1	B	782	PHE	2.2
1	B	518	LEU	2.1
1	B	1857	ASN	2.1
1	B	2065	TRP	2.1
1	B	1600	TYR	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

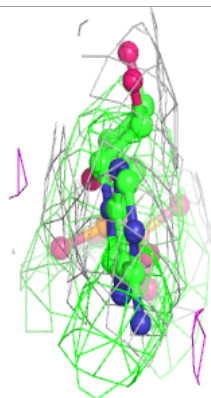
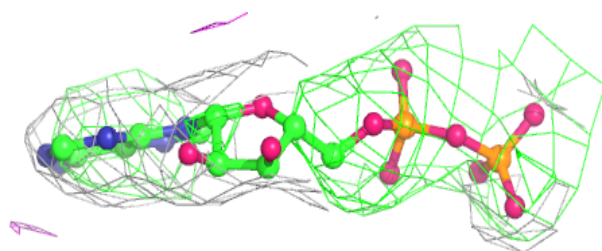
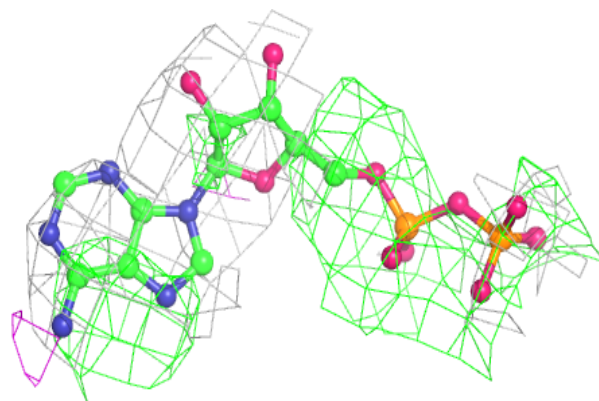
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	B	2201	27/27	0.77	0.48	271,272,275,275	0
3	ADP	B	2202	27/27	0.81	0.37	228,231,231,232	0
4	MG	B	2203	1/1	0.88	0.49	211,211,211,211	0

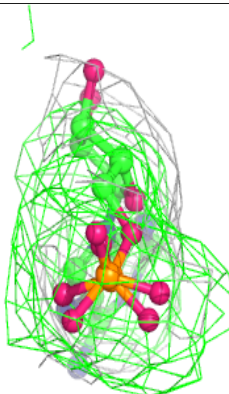
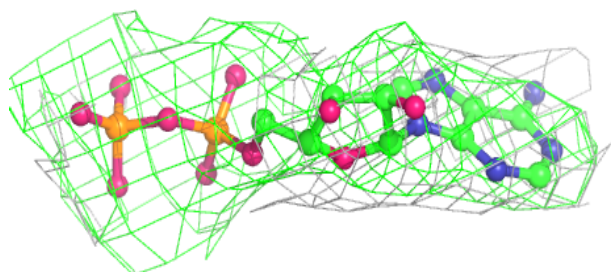
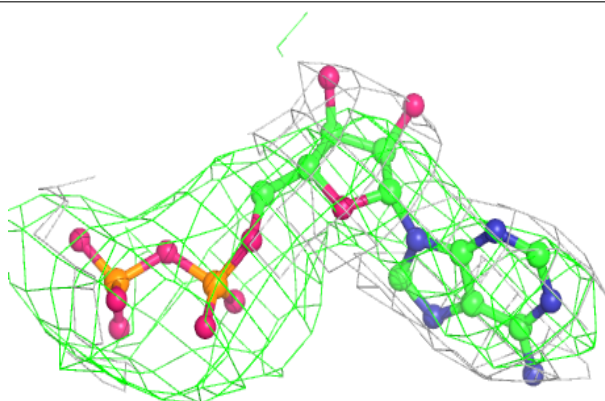
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 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 ADP 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.