



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:19 PM UTC

PDB ID : 4R7Y / pdb_00004r7y
Title : Crystal structure of an active MCM hexamer
Authors : Miller, J.M.; Arachea, B.T.; Epling, L.B.; Enemark, E.J.
Deposited on : 2014-08-28
Resolution : 2.70 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

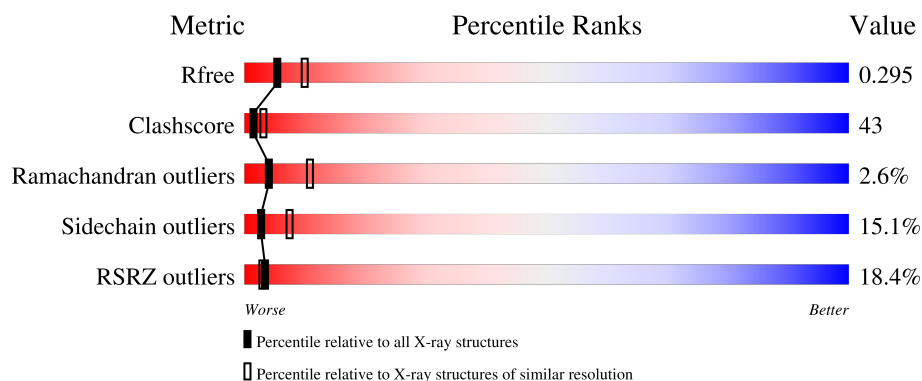
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	613	
1	B	613	

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
5	CL	A	2006	-	-	X	-
5	CL	B	2006	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9494 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.

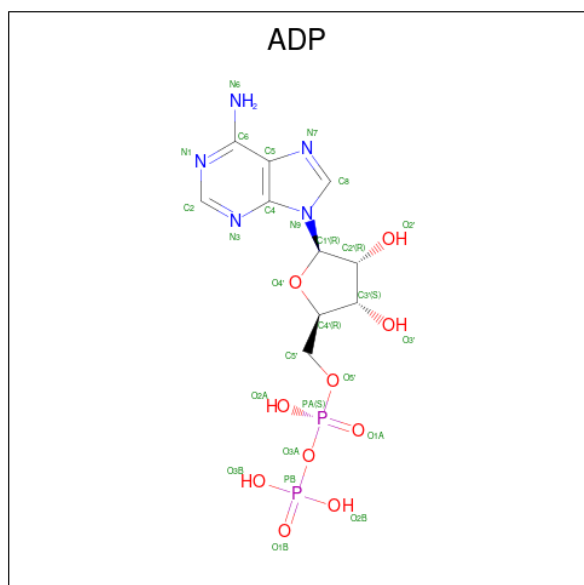
- Molecule 1 is a protein called Minichromosome maintenance protein MCM, Cell division control protein 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4715	3001	822	878	14			
1	B	591	Total	C	N	O	S	0	0	0
			4715	3001	822	878	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9UXG1
A	1	LEU	-	expression tag	UNP Q9UXG1
B	0	SER	-	expression tag	UNP Q9UXG1
B	1	LEU	-	expression tag	UNP Q9UXG1

- 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
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

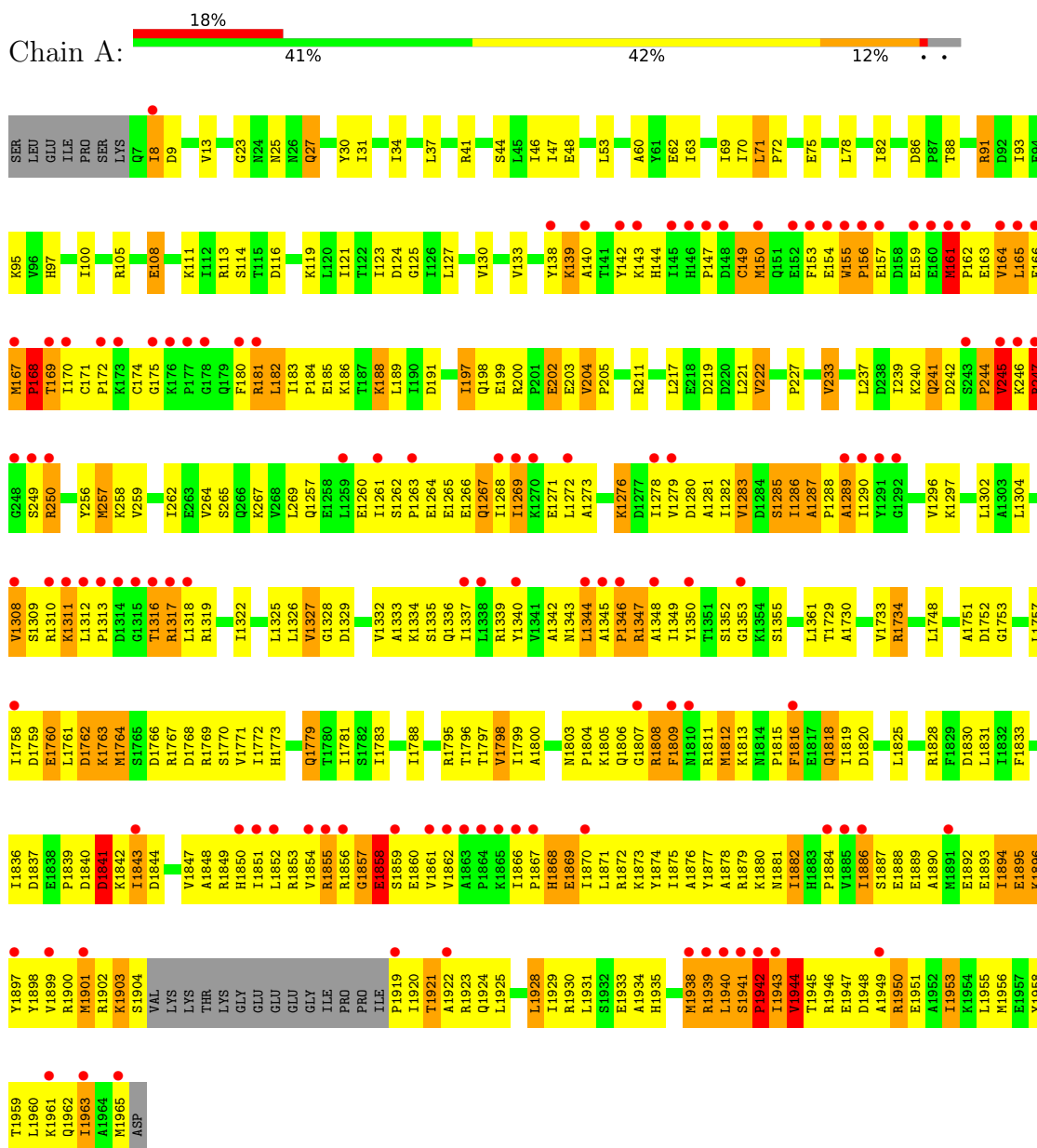
- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl	0	0
			3	3		
5	B	3	Total	Cl	0	0
			3	3		

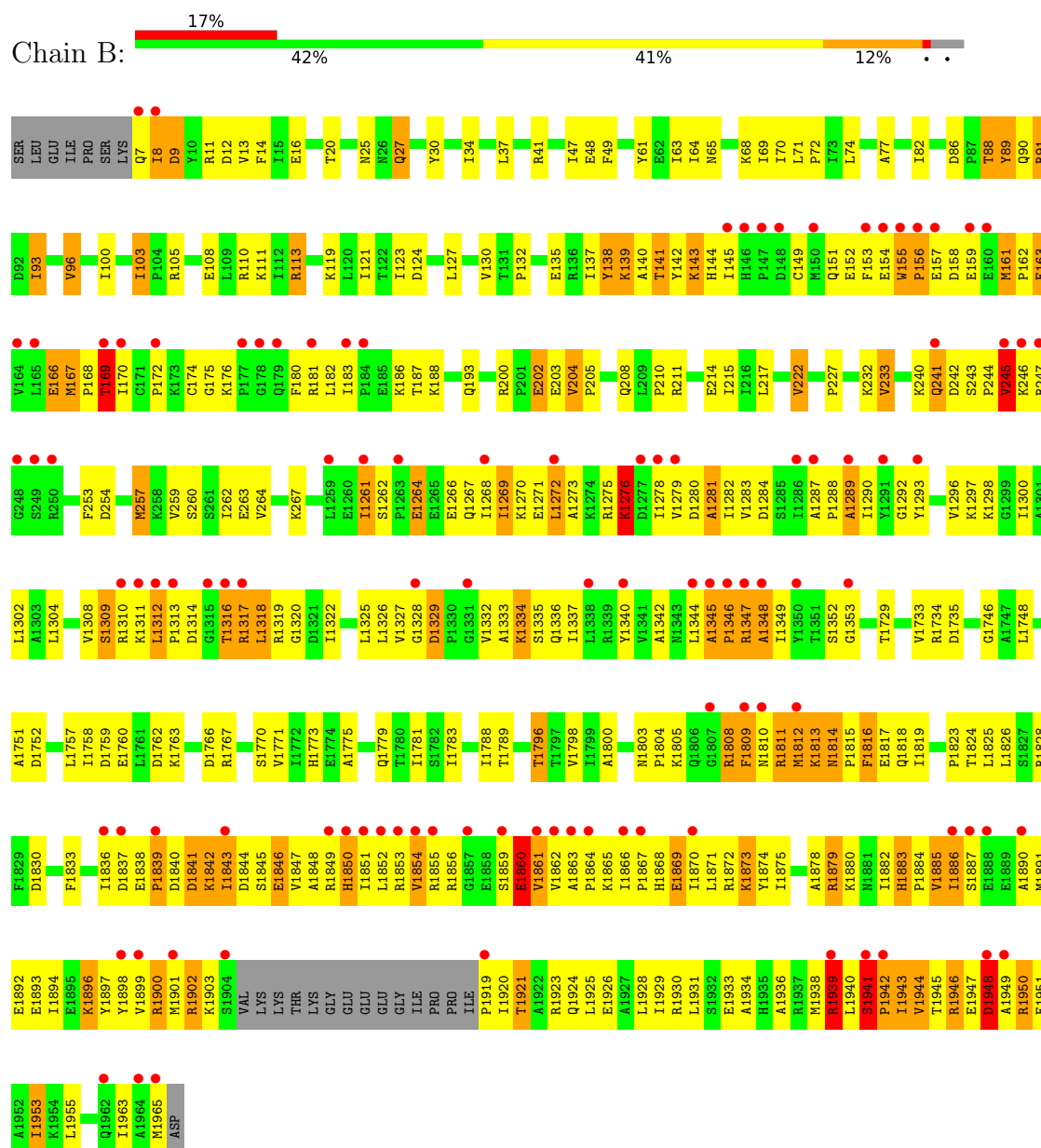
3 Residue-property plots

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

- Molecule 1: Minichromosome maintenance protein MCM, Cell division control protein 21



- Molecule 1: Minichromosome maintenance protein MCM, Cell division control protein 21



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	118.90Å 118.90Å 199.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.83 – 2.70 49.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.7 (49.83-2.70) 89.7 (49.83-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.263 , 0.295 0.263 , 0.295	Depositor DCC
R_{free} test set	1976 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9494	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4816e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ADP, CL, ZN, 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	A	0.59	3/4793 (0.1%)	1.07	25/6476 (0.4%)
1	B	0.59	1/4793 (0.0%)	1.09	30/6476 (0.5%)
All	All	0.59	4/9586 (0.0%)	1.08	55/12952 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	MET	SD-CE	6.39	1.95	1.79
1	A	150	MET	SD-CE	5.78	1.94	1.79
1	B	257	MET	SD-CE	-5.29	1.66	1.79
1	A	257	MET	SD-CE	-5.28	1.66	1.79

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ILE	N-CA-C	-7.83	103.17	110.53
1	B	1816	PHE	N-CA-C	7.59	119.56	111.28
1	A	204	VAL	CA-C-N	7.18	127.58	119.83
1	A	204	VAL	C-N-CA	7.18	127.58	119.83
1	B	1317	ARG	N-CA-C	6.82	119.68	109.25
1	A	1944	VAL	N-CA-C	-6.81	102.63	110.05
1	A	1938	MET	N-CA-C	-6.81	104.45	112.89
1	A	1317	ARG	N-CA-C	6.71	119.52	109.25
1	A	1798	VAL	N-CA-C	6.70	118.12	108.48
1	A	164	VAL	N-CA-C	-6.64	100.39	109.55
1	A	244	PRO	N-CA-C	6.62	121.33	111.41
1	A	204	VAL	N-CA-C	6.50	114.98	107.89
1	A	1816	PHE	N-CA-C	6.50	119.36	111.82
1	A	1344	LEU	N-CA-C	-6.49	105.28	113.72
1	B	1860	GLU	N-CA-C	-6.48	100.24	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1881	ASN	N-CA-C	6.41	121.18	113.23
1	B	259	VAL	N-CA-C	6.41	117.85	109.58
1	A	93	ILE	N-CA-C	6.26	117.04	107.77
1	B	1939	ARG	N-CA-C	-6.16	104.11	111.69
1	B	1345	ALA	CA-C-N	6.14	127.51	119.84
1	B	1345	ALA	C-N-CA	6.14	127.51	119.84
1	A	1287	ALA	CA-C-N	6.11	126.29	119.32
1	A	1287	ALA	C-N-CA	6.11	126.29	119.32
1	B	1348	ALA	N-CA-C	5.95	118.46	109.41
1	B	1788	ILE	N-CA-C	5.92	116.83	108.36
1	B	1883	HIS	CA-C-N	5.89	127.20	119.84
1	B	1883	HIS	C-N-CA	5.89	127.20	119.84
1	B	169	THR	N-CA-C	-5.86	104.25	111.40
1	B	1946	ARG	N-CA-C	-5.86	105.02	111.82
1	B	138	TYR	N-CA-C	-5.86	106.30	113.50
1	B	1798	VAL	N-CA-C	5.85	116.36	108.17
1	B	1943	ILE	N-CA-C	-5.76	100.38	108.27
1	A	149	CYS	N-CA-C	5.71	119.71	111.02
1	A	70	ILE	N-CA-C	5.71	116.45	110.62
1	B	1838	GLU	N-CA-C	-5.67	102.29	110.40
1	B	204	VAL	N-CA-C	5.63	114.03	107.89
1	B	1264	GLU	N-CA-C	-5.52	105.18	111.14
1	B	204	VAL	CA-C-N	5.47	125.48	119.90
1	B	204	VAL	C-N-CA	5.47	125.48	119.90
1	B	93	ILE	N-CA-C	5.45	115.97	108.12
1	A	108	GLU	N-CA-C	-5.45	101.79	109.96
1	B	245	VAL	N-CA-C	5.43	120.63	109.34
1	A	62	GLU	N-CA-C	-5.39	105.51	111.71
1	B	1281	ALA	N-CA-C	-5.37	105.12	110.97
1	A	219	ASP	CB-CA-C	-5.31	110.00	117.23
1	A	95	LYS	N-CA-C	5.28	116.87	108.79
1	B	1276	LYS	N-CA-C	5.26	117.82	111.40
1	B	167	MET	CA-C-N	5.24	125.15	119.76
1	B	167	MET	C-N-CA	5.24	125.15	119.76
1	B	70	ILE	N-CA-C	5.20	115.92	110.62
1	A	1327	VAL	N-CA-C	-5.16	100.98	108.97
1	A	1343	ASN	N-CA-C	-5.11	106.88	113.01
1	B	1312	LEU	CA-C-N	5.10	126.21	119.84
1	B	1312	LEU	C-N-CA	5.10	126.21	119.84
1	A	189	LEU	N-CA-C	5.02	117.75	109.72

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	A	4715	0	4876	442	0
1	B	4715	0	4876	408	0
2	A	27	0	12	3	0
2	B	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	2	0
5	B	3	0	0	2	0
All	All	9494	0	9776	834	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 43.

All (834) 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:1346:PRO:HB3	1:B:1872:ARG:HD3	1.29	1.10
1:A:156:PRO:HB2	1:A:159:GLU:O	1.53	1.07
1:B:1261:ILE:HA	1:B:1873:LYS:HZ1	1.16	1.06
1:A:1878:ALA:HA	1:A:1882:ILE:HD11	1.37	1.05
1:B:1261:ILE:HA	1:B:1873:LYS:NZ	1.73	1.04
1:A:105:ARG:NH1	5:A:2006:CL:CL	2.32	1.00
1:A:1260:GLU:O	1:A:1873:LYS:HE2	1.62	0.99
1:A:1902:ARG:HB3	1:A:1903:LYS:HZ3	1.24	0.98
1:A:1345:ALA:HB1	1:A:1348:ALA:HB3	1.44	0.97
1:A:161:MET:HE1	1:A:165:LEU:HA	1.42	0.97
1:A:1809:PHE:HD1	1:A:1809:PHE:H	1.10	0.96
1:B:105:ARG:NH1	5:B:2006:CL:CL	2.35	0.96
1:B:1949:ALA:O	1:B:1953:ILE:HG22	1.65	0.96
1:B:1311:LYS:HE2	1:B:1317:ARG:HH11	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1809:PHE:H	1:B:1809:PHE:HD1	1.10	0.95
1:B:1894:ILE:HG13	1:B:1928:LEU:HD23	1.49	0.95
1:A:1920:ILE:HG23	1:A:1924:GLN:HG3	1.47	0.94
1:A:1882:ILE:HD13	1:A:1882:ILE:N	1.82	0.92
1:B:156:PRO:HB2	1:B:159:GLU:O	1.67	0.92
1:A:170:ILE:HG23	1:A:175:GLY:O	1.70	0.92
1:B:103:ILE:HD13	1:B:103:ILE:H	1.36	0.90
1:A:162:PRO:HG2	1:A:164:VAL:O	1.70	0.90
1:B:1290:ILE:HD11	1:B:1297:LYS:HE2	1.51	0.90
1:B:1261:ILE:HD13	1:B:1261:ILE:H	1.35	0.90
1:A:1889:GLU:HB3	1:A:1946:ARG:CG	2.02	0.89
1:B:214:GLU:OE2	1:B:240:LYS:HE2	1.74	0.88
1:A:143:LYS:HB2	1:A:183:ILE:HD11	1.52	0.88
1:B:1886:ILE:HD12	1:B:1886:ILE:H	1.39	0.88
1:B:1317:ARG:NH2	1:B:1779:GLN:HG3	1.88	0.87
1:A:1889:GLU:HB3	1:A:1946:ARG:HG2	1.56	0.86
1:B:1863:ALA:HB1	1:B:1864:PRO:HD2	1.58	0.85
1:B:25:ASN:H	1:B:27:GLN:NE2	1.76	0.84
1:B:1317:ARG:HH21	1:B:1779:GLN:HG3	1.42	0.84
1:B:143:LYS:HG3	1:B:152:GLU:HG2	1.60	0.84
1:A:144:HIS:HB3	1:A:149:CYS:SG	2.17	0.83
1:B:1329:ASP:O	1:B:1332:VAL:HG22	1.78	0.83
1:A:1312:LEU:HB3	1:A:1313:PRO:HD2	1.61	0.83
1:B:1329:ASP:OD1	1:B:1808:ARG:HA	1.78	0.82
1:B:1269:ILE:HD11	1:B:1874:TYR:HA	1.62	0.82
1:A:1893:GLU:OE1	1:A:1950:ARG:HD2	1.79	0.82
1:B:1752:ASP:HA	1:B:1796:THR:HG22	1.61	0.82
1:B:1276:LYS:HA	1:B:1276:LYS:HE2	1.62	0.82
1:B:156:PRO:HG3	1:B:161:MET:HG2	1.62	0.82
1:A:1960:LEU:O	1:A:1963:ILE:HG13	1.81	0.81
1:A:41:ARG:NH2	1:A:88:THR:HG22	1.96	0.81
1:B:1281:ALA:HB1	1:B:1866:ILE:HD11	1.62	0.80
1:A:1882:ILE:HD13	1:A:1882:ILE:H	1.40	0.80
1:A:1901:MET:SD	1:A:1920:ILE:HG21	2.21	0.80
1:B:1310:ARG:O	1:B:1318:LEU:HB2	1.81	0.79
1:A:25:ASN:H	1:A:27:GLN:HE21	1.28	0.79
1:B:1317:ARG:HH22	1:B:1779:GLN:HE21	1.30	0.79
1:B:1823:PRO:HA	1:B:1826:LEU:HD12	1.65	0.79
1:A:1760:GLU:HG3	1:A:1763:LYS:CG	2.13	0.79
1:A:1760:GLU:HG3	1:A:1763:LYS:HG3	1.65	0.79
1:B:1946:ARG:HD3	1:B:1950:ARG:HH12	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASN:H	1:B:27:GLN:HE21	1.30	0.79
1:A:249:SER:O	1:A:250:ARG:HG3	1.83	0.78
1:A:1265:GLU:O	1:A:1269:ILE:HG22	1.82	0.78
1:B:86:ASP:OD1	1:B:88:THR:HB	1.82	0.78
1:B:1311:LYS:NZ	1:B:1317:ARG:HB2	1.99	0.78
1:A:1276:LYS:HE2	1:A:1276:LYS:HA	1.65	0.78
1:A:1901:MET:SD	1:A:1920:ILE:HG13	2.24	0.77
1:B:41:ARG:NH2	1:B:88:THR:HG22	1.99	0.77
1:B:1345:ALA:HB1	1:B:1348:ALA:HB3	1.64	0.77
1:B:1810:ASN:HD21	1:B:1836:ILE:CG2	1.97	0.77
1:A:161:MET:HE3	1:A:162:PRO:HD2	1.66	0.77
1:B:1946:ARG:HD3	1:B:1950:ARG:NH1	1.99	0.77
1:A:1878:ALA:O	1:A:1882:ILE:HG12	1.83	0.77
1:B:1311:LYS:HZ3	1:B:1317:ARG:HB2	1.48	0.77
1:B:1815:PRO:HD3	1:B:1965:MET:HE2	1.64	0.77
1:A:1779:GLN:CG	1:A:1795:ARG:HA	2.15	0.77
1:A:1902:ARG:HB3	1:A:1903:LYS:NZ	1.99	0.77
1:A:1752:ASP:HA	1:A:1796:THR:HG22	1.66	0.76
1:B:1850:HIS:O	1:B:1854:VAL:HG23	1.85	0.76
1:B:1336:GLN:HG3	1:B:1340:TYR:HE1	1.51	0.76
1:A:1729:THR:HB	1:A:1781:ILE:HD13	1.66	0.76
1:A:1264:GLU:O	1:A:1268:ILE:HG13	1.86	0.75
1:B:1332:VAL:HG23	1:B:1334:LYS:HD2	1.69	0.75
1:A:1828:ARG:HE	1:A:1923:ARG:NH2	1.83	0.75
1:A:1899:VAL:O	1:A:1903:LYS:HE2	1.86	0.75
1:A:1289:ALA:HB3	1:A:1340:TYR:CE2	2.21	0.75
1:B:1327:VAL:HG13	1:B:1819:ILE:HG21	1.67	0.75
1:A:1345:ALA:CB	1:A:1348:ALA:HB3	2.17	0.75
1:A:1348:ALA:C	1:A:1349:ILE:HD12	2.11	0.74
1:B:1332:VAL:CG2	1:B:1334:LYS:HD2	2.17	0.74
1:A:1280:ASP:O	1:A:1283:VAL:HG13	1.88	0.74
1:B:1336:GLN:HG3	1:B:1340:TYR:CE1	2.23	0.73
1:B:1874:TYR:OH	1:B:1940:LEU:HD11	1.88	0.73
1:A:1278:ILE:HG23	1:A:1279:VAL:H	1.53	0.73
1:B:143:LYS:HB2	1:B:183:ILE:HD11	1.69	0.73
1:A:1839:PRO:HB3	1:B:1902:ARG:HH11	1.53	0.73
1:A:1278:ILE:HG23	1:A:1279:VAL:N	2.04	0.72
1:A:1332:VAL:HG12	1:A:1332:VAL:O	1.88	0.72
1:A:1878:ALA:HA	1:A:1882:ILE:CD1	2.18	0.72
1:A:1878:ALA:CA	1:A:1882:ILE:HD11	2.19	0.72
1:A:1828:ARG:NE	1:A:1923:ARG:HH22	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1289:ALA:HB3	1:A:1340:TYR:HE2	1.56	0.71
1:A:1815:PRO:HG2	1:A:1963:ILE:HG22	1.72	0.71
1:A:1809:PHE:HB2	1:A:1818:GLN:OE1	1.90	0.71
1:B:1901:MET:SD	1:B:1920:ILE:HG13	2.30	0.71
1:A:1261:ILE:HA	1:A:1873:LYS:NZ	2.05	0.71
1:A:211:ARG:NH1	1:B:132:PRO:HA	2.07	0.70
1:B:1919:PRO:HG2	1:B:1920:ILE:H	1.57	0.70
1:B:1809:PHE:HD1	1:B:1809:PHE:N	1.88	0.70
1:B:1843:ILE:HA	1:B:1846:GLU:HG3	1.74	0.70
1:A:156:PRO:HG3	1:A:161:MET:HG2	1.73	0.70
1:A:1869:GLU:HA	1:A:1872:ARG:HH11	1.57	0.70
1:B:1312:LEU:O	1:B:1316:THR:HA	1.92	0.69
1:B:1809:PHE:N	1:B:1809:PHE:CD1	2.60	0.69
1:B:1810:ASN:HD21	1:B:1836:ILE:HG23	1.57	0.69
1:A:171:CYS:HB3	1:A:174:CYS:SG	2.33	0.69
1:A:1779:GLN:HG3	1:A:1795:ARG:HA	1.74	0.69
1:A:1960:LEU:HA	1:A:1963:ILE:HD11	1.74	0.69
1:B:140:ALA:HA	1:B:187:THR:HG23	1.73	0.69
1:B:144:HIS:HB3	1:B:149:CYS:SG	2.33	0.69
1:B:1944:VAL:HG12	1:B:1948:ASP:CB	2.22	0.69
1:A:1871:LEU:O	1:A:1874:TYR:HB3	1.92	0.69
1:A:1939:ARG:HH12	1:A:1948:ASP:CG	2.00	0.69
1:B:1333:ALA:O	1:B:1337:ILE:HG13	1.93	0.69
1:A:1867:PRO:HG2	1:A:1870:ILE:HD12	1.75	0.69
1:A:1886:ILE:HA	1:A:1944:VAL:CG2	2.23	0.69
1:B:1884:PRO:HA	1:B:1942:PRO:HB2	1.75	0.69
1:A:1267:GLN:O	1:A:1271:GLU:HG2	1.92	0.68
1:A:1760:GLU:OE2	1:A:1760:GLU:HA	1.92	0.68
1:A:202:GLU:HG2	1:A:267:LYS:NZ	2.07	0.68
1:A:1773:HIS:HB3	1:A:1828:ARG:HH12	1.58	0.68
1:B:170:ILE:HG23	1:B:175:GLY:O	1.93	0.68
1:B:1288:PRO:C	1:B:1290:ILE:H	2.00	0.68
1:A:1290:ILE:HD11	1:A:1297:LYS:HE2	1.75	0.68
1:B:1871:LEU:O	1:B:1874:TYR:HB3	1.94	0.68
1:B:155:TRP:O	1:B:157:GLU:N	2.27	0.68
1:B:1348:ALA:C	1:B:1349:ILE:HD12	2.19	0.68
1:A:1828:ARG:HE	1:A:1923:ARG:HH22	1.41	0.68
1:B:1316:THR:OG1	1:B:1317:ARG:N	2.25	0.68
1:B:1939:ARG:C	1:B:1940:LEU:HD12	2.18	0.67
1:B:161:MET:HE1	1:B:166:GLU:H	1.60	0.67
1:B:1893:GLU:HG3	1:B:1946:ARG:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG23	1:A:227:PRO:HG3	1.76	0.67
1:A:1929:ILE:O	1:A:1933:GLU:HG3	1.94	0.67
1:A:1287:ALA:O	1:A:1290:ILE:HG12	1.95	0.67
1:B:25:ASN:N	1:B:27:GLN:HE21	1.93	0.67
1:B:1936:ALA:HB2	1:B:1948:ASP:OD1	1.94	0.67
1:A:161:MET:CE	1:A:165:LEU:HD13	2.24	0.67
1:B:1899:VAL:O	1:B:1903:LYS:HE3	1.95	0.67
1:A:202:GLU:HG2	1:A:267:LYS:HZ2	1.59	0.67
1:A:1342:ALA:HA	1:A:1345:ALA:HB2	1.74	0.67
1:A:1308:VAL:HB	1:A:1933:GLU:OE2	1.94	0.67
1:A:1920:ILE:CG2	1:A:1924:GLN:HG3	2.23	0.67
1:B:141:THR:HG22	1:B:183:ILE:HB	1.76	0.67
1:B:1312:LEU:O	1:B:1316:THR:CA	2.43	0.67
1:B:1311:LYS:HE2	1:B:1317:ARG:NH1	2.07	0.67
1:A:1280:ASP:HA	1:A:1283:VAL:CG1	2.25	0.66
1:A:161:MET:CE	1:A:165:LEU:HA	2.23	0.66
1:A:1839:PRO:HB3	1:B:1902:ARG:NH1	2.10	0.66
1:B:242:ASP:O	1:B:244:PRO:HD3	1.95	0.66
1:A:155:TRP:O	1:A:157:GLU:N	2.29	0.66
1:B:1276:LYS:HA	1:B:1276:LYS:CE	2.25	0.66
1:B:167:MET:HE2	1:B:180:PHE:HB2	1.78	0.66
1:B:1327:VAL:CG1	1:B:1819:ILE:HG21	2.26	0.66
1:B:1867:PRO:HB2	1:B:1870:ILE:HB	1.76	0.66
1:B:1280:ASP:O	1:B:1283:VAL:HG22	1.95	0.66
1:B:211:ARG:HG3	1:B:211:ARG:HH11	1.61	0.66
1:A:1809:PHE:CD1	1:A:1809:PHE:N	2.61	0.66
1:B:1812:MET:SD	1:B:1812:MET:N	2.69	0.65
1:B:1943:ILE:HG22	1:B:1944:VAL:O	1.95	0.65
1:A:1928:LEU:HD22	1:A:1956:MET:HE2	1.76	0.65
1:B:1812:MET:H	1:B:1812:MET:HE2	1.61	0.65
1:B:1890:ALA:O	1:B:1894:ILE:HG22	1.97	0.65
1:A:165:LEU:HD12	1:A:166:GLU:N	2.12	0.65
1:A:1939:ARG:C	1:A:1940:LEU:HD12	2.22	0.65
1:B:1941:SER:CB	1:B:1943:ILE:H	2.10	0.65
1:A:143:LYS:HE3	1:A:150:MET:HG3	1.80	0.64
1:B:1748:LEU:O	1:B:1796:THR:HG21	1.97	0.64
1:A:1848:ALA:HB2	1:B:1898:TYR:HD2	1.61	0.64
1:A:1958:TYR:O	1:A:1962:GLN:HG3	1.98	0.64
1:B:1311:LYS:HZ3	1:B:1317:ARG:CB	2.09	0.64
1:A:168:PRO:O	1:A:180:PHE:CE2	2.51	0.64
1:B:1317:ARG:NH2	1:B:1779:GLN:HE21	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1758:ILE:O	1:B:1800:ALA:HA	1.97	0.64
1:A:1949:ALA:O	1:A:1953:ILE:HG22	1.98	0.64
1:A:30:TYR:CE1	1:A:47:ILE:HD13	2.32	0.64
1:A:1850:HIS:O	1:A:1854:VAL:HG23	1.98	0.63
1:B:1729:THR:HB	1:B:1781:ILE:HD13	1.79	0.63
1:B:1767:ARG:HB3	1:B:1767:ARG:CZ	2.26	0.63
1:B:1856:ARG:HB2	1:B:1860:GLU:OE2	1.97	0.63
1:B:155:TRP:O	1:B:156:PRO:C	2.41	0.63
1:B:1292:GLY:O	1:B:1297:LYS:HE3	1.98	0.63
1:A:1285:SER:OG	1:A:1866:ILE:HG13	1.97	0.63
1:B:1886:ILE:HA	1:B:1944:VAL:HG21	1.81	0.63
1:A:1290:ILE:HD11	1:A:1297:LYS:CE	2.29	0.63
1:A:1848:ALA:O	1:A:1852:LEU:HD23	1.98	0.63
1:B:1342:ALA:O	1:B:1345:ALA:HB3	1.98	0.63
1:A:155:TRP:HB3	1:A:156:PRO:CD	2.29	0.63
1:A:161:MET:HE1	1:A:165:LEU:HD13	1.81	0.63
1:B:156:PRO:CG	1:B:161:MET:HG2	2.29	0.63
1:A:1290:ILE:HA	2:A:2001:ADP:N1	2.15	0.62
1:A:1887:SER:HB3	1:A:1944:VAL:O	1.99	0.62
1:B:1729:THR:HG21	1:B:1771:VAL:HG23	1.80	0.62
1:A:1837:ASP:OD2	1:B:1902:ARG:NH2	2.32	0.62
1:A:1758:ILE:O	1:A:1800:ALA:HA	1.99	0.62
1:A:1882:ILE:N	1:A:1882:ILE:CD1	2.56	0.62
1:B:1878:ALA:HA	1:B:1882:ILE:HG12	1.81	0.62
1:A:1329:ASP:OD1	1:A:1808:ARG:HA	1.99	0.62
1:A:1879:ARG:HG2	1:A:1879:ARG:HH11	1.64	0.62
1:A:233:VAL:HB	1:A:257:MET:HE1	1.82	0.62
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.64	0.62
1:A:1959:THR:O	1:A:1962:GLN:HB2	2.00	0.61
1:B:1273:ALA:HA	1:B:1278:ILE:CD1	2.29	0.61
1:B:1856:ARG:HB2	1:B:1860:GLU:CD	2.25	0.61
1:A:167:MET:HB3	1:A:168:PRO:HD2	1.82	0.61
1:A:1281:ALA:HB3	1:A:1866:ILE:HD11	1.83	0.61
1:A:1734:ARG:HG3	1:A:1734:ARG:HH11	1.66	0.61
1:A:119:LYS:HD2	5:A:2006:CL:CL	2.38	0.61
1:B:1273:ALA:HA	1:B:1278:ILE:HD12	1.82	0.61
1:B:1963:ILE:O	1:B:1965:MET:HG3	2.00	0.61
1:A:1840:ASP:HB3	1:A:1843:ILE:HG23	1.83	0.61
1:A:1945:THR:O	1:A:1948:ASP:HB2	2.00	0.61
1:A:169:THR:HB	1:A:170:ILE:HD12	1.83	0.60
1:B:1903:LYS:HE2	1:B:1903:LYS:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1287:ALA:O	1:B:1290:ILE:HG12	2.00	0.60
1:A:116:ASP:HA	1:A:119:LYS:HZ2	1.66	0.60
1:A:1333:ALA:O	1:A:1337:ILE:HG13	2.00	0.60
1:B:49:PHE:CZ	1:B:64:ILE:HD11	2.36	0.60
1:B:1867:PRO:CB	1:B:1870:ILE:HD13	2.31	0.60
1:A:1875:ILE:O	1:A:1878:ALA:HB3	2.01	0.60
1:A:1890:ALA:O	1:A:1894:ILE:HG22	2.02	0.60
1:A:1920:ILE:HG22	1:A:1921:THR:N	2.15	0.60
1:B:1336:GLN:O	1:B:1340:TYR:HD1	1.85	0.60
1:A:1856:ARG:NH1	1:A:1860:GLU:OE1	2.34	0.60
1:A:181:ARG:O	1:A:183:ILE:HD12	2.02	0.60
1:A:1261:ILE:HA	1:A:1873:LYS:HZ3	1.67	0.60
1:B:1864:PRO:HB3	1:B:1868:HIS:CD2	2.37	0.60
1:B:1920:ILE:HG23	1:B:1924:GLN:HG3	1.82	0.60
1:B:88:THR:O	1:B:91:ARG:HG2	2.01	0.59
1:B:1866:ILE:N	1:B:1866:ILE:HD12	2.16	0.59
1:A:1329:ASP:O	1:A:1332:VAL:HG23	2.02	0.59
1:B:168:PRO:O	1:B:180:PHE:CE2	2.55	0.59
1:B:1311:LYS:O	1:B:1312:LEU:HD23	2.02	0.59
1:B:1899:VAL:O	1:B:1903:LYS:HG2	2.01	0.59
1:B:1853:ARG:O	1:B:1856:ARG:HG3	2.02	0.59
1:B:1282:ILE:HD12	1:B:1938:MET:HE2	1.84	0.59
1:A:1897:TYR:CE2	1:A:1901:MET:HE2	2.37	0.59
1:A:1946:ARG:C	1:A:1950:ARG:HE	2.11	0.59
1:B:144:HIS:CE1	1:B:176:LYS:O	2.56	0.59
1:B:1760:GLU:OE2	1:B:1803:ASN:ND2	2.36	0.59
1:B:1332:VAL:HG23	1:B:1334:LYS:CD	2.32	0.59
1:A:142:TYR:OH	1:A:165:LEU:HD11	2.03	0.58
1:A:1311:LYS:C	1:A:1312:LEU:HG	2.28	0.58
1:B:1810:ASN:HD21	1:B:1836:ILE:HG21	1.67	0.58
1:B:1290:ILE:CD1	1:B:1297:LYS:HE2	2.29	0.58
1:B:1811:ARG:CD	1:B:1813:LYS:HB2	2.32	0.58
1:B:141:THR:HG21	1:B:186:LYS:HB2	1.84	0.58
1:A:1317:ARG:NH2	1:A:1779:GLN:HE21	2.00	0.58
1:A:1308:VAL:CG1	1:A:1309:SER:N	2.65	0.58
1:A:1342:ALA:O	1:A:1345:ALA:HB3	2.03	0.58
1:A:1840:ASP:O	1:A:1843:ILE:N	2.35	0.58
1:A:1860:GLU:OE1	1:A:1860:GLU:HA	2.04	0.58
1:A:246:LYS:HG2	1:A:247:ARG:N	2.18	0.58
1:B:1311:LYS:HG2	1:B:1317:ARG:HA	1.85	0.58
1:B:1941:SER:HB2	1:B:1943:ILE:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1813:LYS:HD2	1:B:1813:LYS:N	2.18	0.58
1:B:1896:LYS:O	1:B:1899:VAL:HG12	2.03	0.58
1:A:143:LYS:CB	1:A:183:ILE:HD11	2.30	0.57
1:A:168:PRO:HG2	1:A:180:PHE:CE2	2.39	0.57
1:B:108:GLU:OE2	1:B:111:LYS:HE3	2.04	0.57
1:B:1812:MET:H	1:B:1812:MET:CE	2.16	0.57
1:B:1886:ILE:HA	1:B:1944:VAL:CG2	2.34	0.57
1:A:114:SER:HB3	1:B:135:GLU:OE1	2.05	0.57
1:A:1332:VAL:O	1:A:1333:ALA:HB3	2.04	0.57
1:A:1769:ARG:O	1:A:1772:ILE:HG22	2.03	0.57
1:A:1886:ILE:HA	1:A:1944:VAL:HG21	1.85	0.57
1:B:1900:ARG:HG3	1:B:1900:ARG:HH11	1.68	0.57
1:A:1894:ILE:HG23	1:A:1895:GLU:N	2.20	0.57
1:A:1896:LYS:O	1:A:1899:VAL:HG12	2.05	0.57
1:A:1886:ILE:HA	1:A:1944:VAL:HG23	1.86	0.57
1:A:245:VAL:HG23	1:A:245:VAL:O	2.04	0.57
1:B:1325:LEU:C	1:B:1326:LEU:HD23	2.29	0.57
1:A:1748:LEU:O	1:A:1796:THR:HG21	2.05	0.57
1:B:41:ARG:HH22	1:B:88:THR:HG22	1.69	0.57
1:B:1288:PRO:C	1:B:1290:ILE:N	2.63	0.57
1:A:23:GLY:HA3	1:A:27:GLN:HE22	1.69	0.57
1:A:1902:ARG:O	1:A:1919:PRO:HD2	2.05	0.57
1:B:143:LYS:HB2	1:B:183:ILE:CD1	2.35	0.56
1:B:1284:ASP:O	1:B:1288:PRO:HG3	2.04	0.56
1:B:1902:ARG:HH11	1:B:1902:ARG:HG2	1.70	0.56
1:A:1811:ARG:HD3	1:A:1813:LYS:HG3	1.87	0.56
1:B:1264:GLU:O	1:B:1268:ILE:HG13	2.05	0.56
1:B:1304:LEU:O	1:B:1879:ARG:HD2	2.05	0.56
1:B:1309:SER:HB2	1:B:1320:GLY:HA3	1.86	0.56
1:B:1941:SER:HB2	1:B:1943:ILE:N	2.19	0.56
1:A:125:GLY:HA3	1:A:197:ILE:HD11	1.86	0.56
1:A:1342:ALA:HB2	1:A:1757:LEU:HD12	1.88	0.56
1:B:1773:HIS:HB3	1:B:1828:ARG:NH1	2.21	0.56
1:B:143:LYS:HD2	1:B:152:GLU:OE2	2.06	0.56
1:B:1308:VAL:HG13	1:B:1309:SER:N	2.19	0.56
1:A:1302:LEU:HD22	1:A:1934:ALA:HB3	1.87	0.56
1:B:1284:ASP:CB	1:B:1865:LYS:HG3	2.36	0.56
1:B:1311:LYS:HZ3	1:B:1317:ARG:HD2	1.71	0.56
1:B:1848:ALA:O	1:B:1852:LEU:HD23	2.05	0.56
1:B:1929:ILE:O	1:B:1933:GLU:HG3	2.05	0.56
1:A:41:ARG:HH21	1:A:88:THR:HG22	1.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1302:LEU:HD22	1:A:1934:ALA:CB	2.35	0.56
1:B:1847:VAL:O	1:B:1851:ILE:HG13	2.06	0.56
1:A:116:ASP:HA	1:A:119:LYS:NZ	2.21	0.56
1:A:1279:VAL:O	1:A:1283:VAL:HG12	2.05	0.56
1:A:1288:PRO:C	1:A:1290:ILE:H	2.14	0.56
1:A:1329:ASP:OD2	1:A:1836:ILE:HG23	2.05	0.56
1:B:1261:ILE:H	1:B:1261:ILE:CD1	2.14	0.56
1:B:1278:ILE:CG2	1:B:1279:VAL:N	2.68	0.56
1:A:1812:MET:SD	1:A:1812:MET:N	2.73	0.55
1:A:63:ILE:HD13	1:A:100:ILE:HD13	1.89	0.55
1:A:1939:ARG:NH1	1:A:1948:ASP:OD2	2.39	0.55
1:A:1308:VAL:HG13	1:A:1309:SER:N	2.19	0.55
1:A:1753:GLY:N	1:A:1795:ARG:O	2.38	0.55
1:A:1950:ARG:NH1	1:A:1950:ARG:HG2	2.21	0.55
1:B:1849:ARG:O	1:B:1853:ARG:HG3	2.07	0.55
1:A:1278:ILE:CG2	1:A:1279:VAL:H	2.18	0.55
1:A:1760:GLU:HG3	1:A:1763:LYS:HG2	1.88	0.55
1:B:1882:ILE:HG22	1:B:1884:PRO:HD3	1.89	0.55
1:A:202:GLU:CD	1:A:202:GLU:H	2.14	0.55
1:A:156:PRO:CG	1:A:161:MET:HG2	2.37	0.55
1:B:7:GLN:HG2	1:B:8:ILE:N	2.21	0.55
1:B:161:MET:HE3	1:B:162:PRO:HD2	1.89	0.55
1:B:1289:ALA:HB3	1:B:1340:TYR:CE2	2.41	0.55
1:A:1273:ALA:HB1	1:A:1940:LEU:HD13	1.89	0.55
1:A:1767:ARG:HB3	1:A:1767:ARG:CZ	2.37	0.55
1:B:1328:GLY:O	1:B:1804:PRO:HD3	2.07	0.55
1:A:1296:VAL:HG22	1:A:1833:PHE:CD2	2.42	0.54
1:A:1897:TYR:CZ	1:A:1901:MET:HE2	2.42	0.54
1:A:233:VAL:HG12	1:A:257:MET:HE3	1.89	0.54
1:A:1840:ASP:O	1:A:1841:ASP:C	2.50	0.54
1:B:1901:MET:HG3	1:B:1920:ILE:HG13	1.88	0.54
1:A:1760:GLU:OE2	1:A:1803:ASN:ND2	2.40	0.54
1:B:202:GLU:HG2	1:B:267:LYS:NZ	2.21	0.54
1:A:217:LEU:CD2	1:A:259:VAL:HG21	2.37	0.54
1:A:1856:ARG:O	1:A:1857:GLY:O	2.26	0.54
1:B:63:ILE:HG21	1:B:100:ILE:HD13	1.89	0.54
1:A:1278:ILE:CG2	1:A:1279:VAL:N	2.71	0.54
1:A:1941:SER:CB	1:A:1943:ILE:H	2.20	0.54
1:B:155:TRP:CH2	1:B:168:PRO:HB3	2.43	0.54
1:B:1325:LEU:O	1:B:1326:LEU:HD23	2.07	0.54
1:B:1853:ARG:HD3	1:B:1856:ARG:HH21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1860:GLU:OE1	1:A:1860:GLU:CA	2.56	0.54
1:A:1894:ILE:HD11	1:A:1925:LEU:HD12	1.90	0.54
1:B:1267:GLN:O	1:B:1271:GLU:HG2	2.07	0.54
1:B:1809:PHE:HB2	1:B:1818:GLN:CD	2.33	0.54
1:A:1855:ARG:HD3	1:B:1318:LEU:HD11	1.88	0.54
1:B:1332:VAL:O	1:B:1333:ALA:HB3	2.08	0.54
1:A:88:THR:O	1:A:91:ARG:HG3	2.08	0.54
1:A:250:ARG:NE	1:B:163:GLU:HG3	2.22	0.54
1:B:181:ARG:O	1:B:183:ILE:HD12	2.08	0.54
1:B:1944:VAL:HG12	1:B:1948:ASP:CG	2.33	0.54
1:A:71:LEU:O	1:A:75:GLU:HG3	2.08	0.54
1:A:183:ILE:HG22	1:A:186:LYS:H	1.72	0.54
1:B:144:HIS:HE1	1:B:176:LYS:O	1.91	0.54
1:B:1288:PRO:O	1:B:1290:ILE:N	2.41	0.53
1:B:1901:MET:CG	1:B:1920:ILE:HG13	2.38	0.53
1:A:1853:ARG:HD3	1:A:1856:ARG:NH2	2.24	0.53
1:B:1269:ILE:HG12	1:B:1874:TYR:HD1	1.73	0.53
1:A:30:TYR:O	1:A:34:ILE:HG13	2.07	0.53
1:A:1809:PHE:HD1	1:A:1809:PHE:N	1.89	0.53
1:A:1896:LYS:HE3	1:A:1900:ARG:HG3	1.90	0.53
1:B:1830:ASP:CG	1:B:1930:ARG:HH21	2.17	0.53
1:A:1929:ILE:HD12	1:A:1929:ILE:N	2.24	0.53
1:B:1284:ASP:HB3	1:B:1865:LYS:HG3	1.88	0.53
1:B:1819:ILE:HD12	1:B:1819:ILE:O	2.07	0.53
1:A:1813:LYS:O	1:A:1965:MET:HE1	2.09	0.53
1:B:1261:ILE:HA	1:B:1873:LYS:HZ3	1.70	0.53
1:A:1853:ARG:CD	1:A:1856:ARG:NH2	2.72	0.53
1:B:1939:ARG:HH21	1:B:1947:GLU:HB2	1.74	0.53
1:A:155:TRP:HB3	1:A:156:PRO:HD2	1.90	0.53
1:B:1261:ILE:HG22	1:B:1873:LYS:HZ3	1.73	0.53
1:B:1887:SER:HG	1:B:1943:ILE:HG22	1.74	0.53
1:B:262:ILE:HG23	1:B:262:ILE:O	2.09	0.53
1:A:108:GLU:OE2	1:A:111:LYS:HE3	2.08	0.52
1:B:155:TRP:CZ3	1:B:168:PRO:HB3	2.44	0.52
1:B:1298:LYS:HG2	1:B:1955:LEU:HD22	1.91	0.52
1:A:1901:MET:O	1:A:1904:SER:HB3	2.08	0.52
1:B:143:LYS:CG	1:B:152:GLU:HG2	2.37	0.52
1:B:1884:PRO:CA	1:B:1942:PRO:HB2	2.37	0.52
1:A:1322:ILE:HD13	1:A:1931:LEU:HD23	1.91	0.52
1:B:1290:ILE:HG13	1:B:1290:ILE:O	2.07	0.52
1:B:1302:LEU:HD22	1:B:1934:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1842:LYS:O	1:B:1846:GLU:HG2	2.09	0.52
1:B:1948:ASP:O	1:B:1949:ALA:C	2.52	0.52
1:A:250:ARG:CZ	1:B:163:GLU:HG3	2.39	0.52
1:A:1311:LYS:CD	1:A:1317:ARG:HB2	2.39	0.52
1:A:1779:GLN:HG2	1:A:1795:ARG:HG2	1.91	0.52
1:B:1281:ALA:CB	1:B:1866:ILE:HD11	2.37	0.52
1:A:183:ILE:HD12	1:A:183:ILE:N	2.25	0.52
1:A:1261:ILE:HA	1:A:1873:LYS:CE	2.39	0.52
1:A:1950:ARG:HG2	1:A:1950:ARG:HH11	1.74	0.52
1:B:140:ALA:O	1:B:154:GLU:HA	2.10	0.52
1:A:133:VAL:HG22	1:A:222:VAL:HG13	1.92	0.52
1:A:155:TRP:O	1:A:156:PRO:C	2.51	0.52
1:A:1771:VAL:HG12	1:A:1771:VAL:O	2.10	0.52
1:A:1897:TYR:CG	1:A:1953:ILE:HD12	2.45	0.52
1:A:1902:ARG:CB	1:A:1903:LYS:HZ3	2.11	0.52
1:A:1941:SER:HB2	1:A:1943:ILE:N	2.25	0.52
1:B:155:TRP:HB3	1:B:156:PRO:CD	2.39	0.52
1:A:23:GLY:HA3	1:A:27:GLN:NE2	2.24	0.52
1:A:262:ILE:HG23	1:A:262:ILE:O	2.09	0.52
1:A:105:ARG:HH12	1:A:119:LYS:HZ3	1.58	0.52
1:A:170:ILE:HG23	1:A:175:GLY:C	2.35	0.52
1:B:153:PHE:HZ	1:B:168:PRO:HG3	1.75	0.52
1:B:1903:LYS:HE2	1:B:1903:LYS:CA	2.40	0.52
1:A:1281:ALA:O	1:A:1285:SER:OG	2.23	0.51
1:A:1855:ARG:HG2	1:B:1929:ILE:HG21	1.91	0.51
1:B:1261:ILE:HG12	1:B:1261:ILE:O	2.10	0.51
1:A:142:TYR:CE1	1:A:167:MET:HE2	2.46	0.51
1:A:1339:ARG:HG2	1:A:1350:TYR:CE2	2.45	0.51
1:A:1899:VAL:HG13	1:A:1900:ARG:N	2.25	0.51
1:B:100:ILE:HG22	1:B:103:ILE:HG23	1.92	0.51
1:B:1278:ILE:HG23	1:B:1279:VAL:N	2.25	0.51
1:B:9:ASP:OD2	1:B:11:ARG:HB2	2.09	0.51
1:A:1325:LEU:C	1:A:1326:LEU:HD23	2.35	0.51
1:A:161:MET:HE1	1:A:165:LEU:CA	2.28	0.51
1:B:1283:VAL:HG23	1:B:1284:ASP:N	2.26	0.51
1:A:1346:PRO:C	1:A:1347:ARG:HG3	2.34	0.51
1:B:1289:ALA:CB	1:B:1340:TYR:CE2	2.94	0.51
1:B:14:PHE:CE2	1:B:74:LEU:HB3	2.45	0.51
1:B:1317:ARG:HH11	1:B:1317:ARG:HG3	1.76	0.51
1:B:1322:ILE:HD13	1:B:1931:LEU:HD23	1.93	0.51
1:A:1960:LEU:HA	1:A:1963:ILE:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:MET:HE1	1:A:165:LEU:CD1	2.40	0.51
1:A:240:LYS:HB3	1:A:256:TYR:CE1	2.45	0.51
1:A:1325:LEU:O	1:A:1326:LEU:HD23	2.10	0.51
1:A:1898:TYR:CE1	1:A:1902:ARG:HD2	2.46	0.51
1:A:155:TRP:CB	1:A:156:PRO:CD	2.89	0.51
1:A:1296:VAL:HA	1:A:1833:PHE:CE2	2.45	0.51
1:A:1920:ILE:CG2	1:A:1921:THR:N	2.74	0.51
1:B:193:GLN:HB2	1:B:222:VAL:HG22	1.93	0.51
1:A:69:ILE:O	1:A:72:PRO:HD2	2.11	0.50
1:B:1317:ARG:NH1	1:B:1317:ARG:HG3	2.26	0.50
1:B:1939:ARG:HG3	1:B:1939:ARG:HH11	1.76	0.50
1:A:1852:LEU:HD11	1:B:1894:ILE:HD13	1.91	0.50
1:B:202:GLU:CD	1:B:202:GLU:H	2.18	0.50
1:B:244:PRO:O	1:B:246:LYS:N	2.39	0.50
1:B:1864:PRO:HB2	1:B:1866:ILE:O	2.11	0.50
1:A:41:ARG:HH22	1:A:88:THR:HG22	1.75	0.50
1:B:241:GLN:NE2	1:B:253:PHE:CE2	2.80	0.50
1:B:1342:ALA:HB2	1:B:1757:LEU:HD12	1.92	0.50
1:A:161:MET:HE3	1:A:162:PRO:CD	2.39	0.50
1:A:1317:ARG:O	1:A:1317:ARG:HG3	2.11	0.50
1:A:1282:ILE:HD12	1:A:1938:MET:CE	2.41	0.50
1:A:1816:PHE:O	1:A:1819:ILE:HG12	2.11	0.50
1:A:1844:ASP:OD2	1:B:1902:ARG:HD3	2.12	0.50
1:A:1840:ASP:O	1:A:1842:LYS:N	2.45	0.50
1:B:1773:HIS:CD2	1:B:1828:ARG:NH1	2.80	0.50
1:A:240:LYS:HG3	1:A:241:GLN:N	2.26	0.50
1:A:1840:ASP:HB3	1:A:1843:ILE:CG2	2.42	0.50
1:A:1943:ILE:HG22	1:A:1944:VAL:O	2.11	0.50
1:B:1322:ILE:HG23	1:B:1830:ASP:CG	2.36	0.50
1:A:211:ARG:NH1	1:A:211:ARG:HG3	2.27	0.50
1:A:1773:HIS:HB3	1:A:1828:ARG:NH1	2.24	0.50
1:A:1920:ILE:HG23	1:A:1924:GLN:CG	2.33	0.50
1:B:41:ARG:HH21	1:B:88:THR:HG22	1.77	0.50
1:B:1853:ARG:HD3	1:B:1856:ARG:NH2	2.27	0.50
1:B:1293:TYR:HB3	1:B:1296:VAL:HB	1.93	0.49
1:B:139:LYS:NZ	1:B:156:PRO:O	2.45	0.49
1:B:181:ARG:O	1:B:183:ILE:CD1	2.59	0.49
1:B:1332:VAL:HG12	1:B:1837:ASP:HB3	1.94	0.49
1:A:1304:LEU:O	1:A:1879:ARG:HD2	2.12	0.49
1:A:1759:ASP:OD1	1:A:1760:GLU:N	2.46	0.49
1:A:1761:LEU:HD11	1:A:1764:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PRO:CD	1:B:161:MET:HG2	2.43	0.49
1:A:1752:ASP:CA	1:A:1796:THR:HG22	2.38	0.49
1:A:1767:ARG:HG3	1:A:1767:ARG:HH11	1.77	0.49
1:A:1848:ALA:HB2	1:B:1898:TYR:CD2	2.46	0.49
1:A:1869:GLU:HA	1:A:1872:ARG:NH1	2.26	0.49
1:B:30:TYR:CE1	1:B:47:ILE:HD13	2.48	0.49
1:B:156:PRO:CB	1:B:159:GLU:O	2.52	0.49
1:B:1312:LEU:O	1:B:1316:THR:N	2.45	0.49
1:A:1290:ILE:HG13	1:A:1290:ILE:O	2.10	0.49
1:B:1329:ASP:OD1	1:B:1808:ARG:CA	2.54	0.49
1:B:1869:GLU:HA	1:B:1872:ARG:HH11	1.78	0.49
1:B:1939:ARG:HG3	1:B:1939:ARG:NH1	2.27	0.49
1:A:246:LYS:HG2	1:A:247:ARG:H	1.75	0.49
1:B:167:MET:HB2	1:B:168:PRO:HD2	1.95	0.49
1:B:1293:TYR:O	1:B:1297:LYS:HG3	2.13	0.49
1:A:153:PHE:CD2	1:A:172:PRO:HG3	2.48	0.49
1:A:1868:HIS:O	1:A:1871:LEU:N	2.43	0.49
1:B:1266:GLU:O	1:B:1269:ILE:HG22	2.12	0.49
1:B:1816:PHE:O	1:B:1819:ILE:HG13	2.13	0.49
1:A:161:MET:HE1	1:A:166:GLU:H	1.77	0.48
1:A:1807:GLY:O	1:A:1808:ARG:C	2.56	0.48
1:A:1879:ARG:HG2	1:A:1879:ARG:NH1	2.27	0.48
1:A:1886:ILE:H	1:A:1886:ILE:HD12	1.78	0.48
1:B:155:TRP:O	1:B:157:GLU:HG3	2.13	0.48
1:A:1282:ILE:HD12	1:A:1938:MET:HE2	1.94	0.48
1:A:1322:ILE:O	1:A:1797:THR:HG23	2.13	0.48
1:B:1867:PRO:HB3	1:B:1870:ILE:HD13	1.95	0.48
1:B:1853:ARG:C	1:B:1855:ARG:H	2.22	0.48
1:A:1312:LEU:O	1:A:1316:THR:HA	2.12	0.48
1:B:182:LEU:C	1:B:183:ILE:HD12	2.39	0.48
1:A:44:SER:HA	1:A:97:HIS:O	2.13	0.48
1:A:168:PRO:HG2	1:A:180:PHE:CZ	2.49	0.48
1:A:200:ARG:O	1:A:203:GLU:HG2	2.14	0.48
1:B:1938:MET:O	1:B:1940:LEU:HD12	2.14	0.48
1:A:1311:LYS:HA	1:A:1317:ARG:HA	1.95	0.48
1:A:1319:ARG:O	1:A:1930:ARG:HD3	2.14	0.48
1:A:1730:ALA:CB	1:A:1783:ILE:HD11	2.43	0.48
1:A:1856:ARG:HG3	1:A:1860:GLU:OE2	2.14	0.48
1:B:1939:ARG:HH11	1:B:1939:ARG:CG	2.26	0.48
1:A:1804:PRO:CG	1:A:1807:GLY:O	2.62	0.48
1:A:1889:GLU:HB3	1:A:1946:ARG:HG3	1.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HD3	5:B:2006:CL:CL	2.51	0.48
1:B:1345:ALA:CB	1:B:1348:ALA:HB3	2.38	0.48
1:B:1867:PRO:HB2	1:B:1870:ILE:HD13	1.95	0.48
1:A:155:TRP:HA	1:A:155:TRP:CE3	2.49	0.48
1:A:1261:ILE:HD11	1:A:1880:LYS:HE2	1.96	0.48
1:B:211:ARG:HG3	1:B:211:ARG:NH1	2.26	0.48
1:B:1312:LEU:HB3	1:B:1313:PRO:HD2	1.95	0.48
1:B:1804:PRO:O	1:B:1805:LYS:C	2.56	0.48
1:B:1879:ARG:HH11	1:B:1879:ARG:HG2	1.77	0.48
1:B:1936:ALA:O	1:B:1939:ARG:HB2	2.14	0.48
1:A:1350:TYR:CD1	1:A:1350:TYR:C	2.92	0.48
1:A:1939:ARG:NH2	1:A:1945:THR:OG1	2.46	0.48
1:B:103:ILE:H	1:B:103:ILE:CD1	2.16	0.48
1:B:1945:THR:O	1:B:1948:ASP:HB2	2.13	0.48
1:A:171:CYS:CB	1:A:174:CYS:SG	2.99	0.47
1:A:1853:ARG:O	1:A:1856:ARG:HG2	2.13	0.47
1:A:1346:PRO:HG2	1:A:1347:ARG:HG3	1.95	0.47
1:A:1898:TYR:CE2	1:A:1925:LEU:HD22	2.49	0.47
1:B:1948:ASP:O	1:B:1951:GLU:N	2.46	0.47
1:A:165:LEU:HD12	1:A:165:LEU:C	2.39	0.47
1:A:1839:PRO:HA	1:A:1844:ASP:OD1	2.13	0.47
1:B:1828:ARG:HE	1:B:1923:ARG:NH2	2.13	0.47
1:A:1311:LYS:HD3	1:A:1317:ARG:HB2	1.96	0.47
1:B:1853:ARG:C	1:B:1855:ARG:N	2.70	0.47
1:A:8:ILE:CG1	1:A:9:ASP:N	2.76	0.47
1:A:1847:VAL:O	1:A:1851:ILE:HG13	2.14	0.47
1:A:171:CYS:O	1:A:175:GLY:N	2.42	0.47
1:A:1257:GLN:O	1:A:1257:GLN:HG3	2.14	0.47
1:A:1262:SER:HB3	1:A:1265:GLU:OE2	2.14	0.47
1:A:1263:PRO:HA	1:A:1266:GLU:HB3	1.95	0.47
1:A:1278:ILE:HD11	1:A:1874:TYR:OH	2.14	0.47
1:A:1332:VAL:O	1:A:1332:VAL:CG1	2.59	0.47
1:A:1922:ALA:O	1:A:1925:LEU:HB3	2.15	0.47
1:B:65:ASN:ND2	1:B:263:GLU:HG3	2.30	0.47
1:B:1853:ARG:O	1:B:1855:ARG:N	2.48	0.47
1:A:1276:LYS:HA	1:A:1276:LYS:CE	2.30	0.47
1:A:1311:LYS:HD2	1:A:1317:ARG:NH1	2.30	0.47
1:A:1751:ALA:O	1:A:1752:ASP:C	2.57	0.47
1:B:1311:LYS:HG2	1:B:1317:ARG:CA	2.44	0.47
1:B:1346:PRO:HG2	1:B:1347:ARG:N	2.30	0.47
1:B:1815:PRO:HG3	1:B:1963:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1840:ASP:HB3	1:B:1843:ILE:CG2	2.45	0.47
1:B:1882:ILE:CG2	1:B:1942:PRO:HB3	2.45	0.47
1:A:239:ILE:O	1:A:239:ILE:HG13	2.15	0.47
1:A:1815:PRO:HG3	1:A:1965:MET:HE2	1.96	0.47
1:A:1853:ARG:HD3	1:A:1856:ARG:HH21	1.80	0.47
1:B:153:PHE:CZ	1:B:168:PRO:HG3	2.50	0.47
1:A:1856:ARG:O	1:A:1860:GLU:OE2	2.33	0.47
1:A:1925:LEU:O	1:A:1929:ILE:HD13	2.15	0.47
1:A:1928:LEU:HD22	1:A:1956:MET:CE	2.42	0.47
1:B:145:ILE:O	1:B:145:ILE:HG22	2.15	0.47
1:A:1276:LYS:HE2	1:A:1276:LYS:CA	2.40	0.46
1:B:137:ILE:HG23	1:B:187:THR:CG2	2.45	0.46
1:B:1319:ARG:O	1:B:1930:ARG:HD3	2.15	0.46
1:A:1310:ARG:HB3	1:A:1312:LEU:HD11	1.96	0.46
1:B:103:ILE:HD13	1:B:103:ILE:N	2.15	0.46
1:B:1813:LYS:O	1:B:1965:MET:HE1	2.15	0.46
1:B:1940:LEU:O	1:B:1941:SER:C	2.58	0.46
1:A:164:VAL:CG2	1:A:244:PRO:HB2	2.46	0.46
1:A:1804:PRO:HG2	1:A:1807:GLY:O	2.15	0.46
1:A:1843:ILE:HG13	1:A:1844:ASP:N	2.30	0.46
1:B:1920:ILE:CG2	1:B:1921:THR:N	2.78	0.46
1:B:1939:ARG:O	1:B:1940:LEU:HB2	2.15	0.46
1:A:1779:GLN:HG2	1:A:1795:ARG:HA	1.97	0.46
1:B:9:ASP:O	1:B:9:ASP:OD1	2.34	0.46
1:B:155:TRP:CG	1:B:156:PRO:N	2.82	0.46
1:B:1810:ASN:O	1:B:1811:ARG:C	2.58	0.46
1:A:185:GLU:H	1:A:185:GLU:CD	2.24	0.46
1:A:1311:LYS:HD2	1:A:1317:ARG:HB2	1.98	0.46
1:A:1761:LEU:CD1	1:A:1764:MET:HE2	2.46	0.46
1:A:1867:PRO:CG	1:A:1870:ILE:HD12	2.45	0.46
1:B:16:GLU:O	1:B:20:THR:OG1	2.34	0.46
1:B:155:TRP:CB	1:B:156:PRO:CD	2.94	0.46
1:A:37:LEU:C	1:A:37:LEU:HD23	2.41	0.46
1:A:182:LEU:O	1:A:184:PRO:HD3	2.16	0.46
1:A:233:VAL:CG1	1:A:257:MET:HE3	2.45	0.46
1:A:1945:THR:O	1:A:1946:ARG:C	2.58	0.46
1:B:1317:ARG:NH2	1:B:1779:GLN:CG	2.72	0.46
1:A:1853:ARG:HA	1:A:1856:ARG:HG2	1.98	0.46
1:B:71:LEU:HB3	1:B:72:PRO:HD3	1.98	0.46
1:A:1342:ALA:C	1:A:1345:ALA:H	2.24	0.46
1:A:1288:PRO:O	1:A:1290:ILE:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:TYR:HD1	1:B:64:ILE:HD12	1.81	0.46
1:B:65:ASN:OD1	1:B:232:LYS:HD2	2.16	0.46
1:A:25:ASN:H	1:A:27:GLN:NE2	2.05	0.45
1:A:1798:VAL:O	1:A:1799:ILE:HD13	2.17	0.45
1:B:1269:ILE:HG22	1:B:1270:LYS:N	2.31	0.45
1:A:1272:LEU:HD12	1:A:1272:LEU:H	1.81	0.45
1:A:1317:ARG:HH21	1:A:1779:GLN:HE21	1.62	0.45
1:B:1352:SER:OG	1:B:1353:GLY:N	2.50	0.45
1:B:1735:ASP:OD1	1:B:1735:ASP:C	2.59	0.45
1:A:198:GLN:HG3	1:A:199:GLU:O	2.16	0.45
1:A:1893:GLU:HG2	1:A:1946:ARG:NH2	2.31	0.45
1:A:1945:THR:O	1:A:1948:ASP:N	2.50	0.45
1:A:221:LEU:O	1:A:222:VAL:C	2.60	0.45
1:B:88:THR:O	1:B:91:ARG:CG	2.64	0.45
1:A:123:ILE:HG22	1:A:124:ASP:N	2.32	0.45
1:A:258:LYS:HD2	1:A:258:LYS:HA	1.78	0.45
1:A:1946:ARG:HB3	1:A:1950:ARG:NE	2.32	0.45
1:A:1951:GLU:OE1	1:A:1951:GLU:HA	2.17	0.45
1:B:1296:VAL:HG22	1:B:1833:PHE:CD2	2.51	0.45
1:B:1751:ALA:O	1:B:1752:ASP:C	2.58	0.45
1:A:217:LEU:HD23	1:A:259:VAL:HG21	1.99	0.45
1:A:1353:GLY:N	1:A:1759:ASP:O	2.50	0.45
1:B:123:ILE:HG22	1:B:124:ASP:N	2.31	0.45
1:B:1272:LEU:O	1:B:1275:ARG:HB3	2.16	0.45
1:B:1760:GLU:CG	1:B:1763:LYS:HD2	2.46	0.45
1:A:1729:THR:OG1	1:A:1730:ALA:N	2.48	0.45
1:A:1752:ASP:HA	1:A:1796:THR:CG2	2.44	0.45
1:A:1779:GLN:HG2	1:A:1795:ARG:CG	2.47	0.45
1:A:1871:LEU:HD12	1:A:1874:TYR:HB3	1.99	0.45
1:B:202:GLU:HG2	1:B:267:LYS:HZ2	1.80	0.45
1:B:1900:ARG:HH11	1:B:1900:ARG:CG	2.30	0.45
1:B:1946:ARG:O	1:B:1950:ARG:HB2	2.17	0.45
1:A:1858:GLU:O	1:A:1859:SER:HB3	2.16	0.45
1:A:1866:ILE:HG22	1:A:1867:PRO:CD	2.46	0.45
1:A:1956:MET:O	1:A:1959:THR:OG1	2.28	0.45
1:B:200:ARG:HB2	1:B:203:GLU:HG2	1.99	0.45
1:B:1276:LYS:HE2	1:B:1276:LYS:CA	2.41	0.45
1:A:1260:GLU:OE2	1:A:1260:GLU:HA	2.17	0.45
1:A:1831:LEU:HD11	1:A:1955:LEU:HD23	1.99	0.45
1:B:37:LEU:HD23	1:B:37:LEU:C	2.42	0.45
1:B:1760:GLU:OE2	1:B:1760:GLU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1844:ASP:OD2	1:B:1902:ARG:NH1	2.50	0.45
1:A:1897:TYR:CE1	1:A:1901:MET:HB3	2.52	0.45
1:B:1308:VAL:CG1	1:B:1309:SER:N	2.80	0.45
1:A:86:ASP:OD1	1:A:88:THR:HB	2.17	0.44
1:A:1946:ARG:CB	1:A:1950:ARG:HE	2.30	0.44
1:B:25:ASN:CA	1:B:27:GLN:HE21	2.29	0.44
1:B:174:CYS:SG	1:B:176:LYS:N	2.81	0.44
1:A:242:ASP:O	1:A:244:PRO:HD3	2.18	0.44
1:A:1760:GLU:OE1	1:A:1763:LYS:HE3	2.17	0.44
1:A:1950:ARG:O	1:A:1953:ILE:HG23	2.17	0.44
1:B:88:THR:C	1:B:90:GLN:N	2.75	0.44
1:B:1843:ILE:HG13	1:B:1844:ASP:N	2.30	0.44
1:B:1897:TYR:CE1	1:B:1901:MET:HB3	2.52	0.44
1:B:1921:THR:H	1:B:1924:GLN:HG3	1.82	0.44
1:A:1261:ILE:HG23	1:A:1873:LYS:HZ1	1.83	0.44
1:A:1346:PRO:HG2	1:A:1347:ARG:N	2.32	0.44
1:A:1876:ALA:O	1:A:1877:TYR:C	2.60	0.44
1:B:1775:ALA:O	1:B:1779:GLN:HA	2.17	0.44
1:B:1869:GLU:OE1	1:B:1869:GLU:N	2.45	0.44
1:B:108:GLU:HB2	1:B:111:LYS:HG3	1.99	0.44
1:B:153:PHE:CD2	1:B:172:PRO:HG3	2.53	0.44
1:A:1262:SER:HB3	1:A:1265:GLU:CD	2.42	0.44
1:A:1262:SER:HB3	1:A:1265:GLU:HB2	2.00	0.44
1:A:1730:ALA:HB3	1:A:1783:ILE:HD11	1.99	0.44
1:A:1282:ILE:HG12	1:A:1866:ILE:HD12	2.00	0.44
1:A:1334:LYS:HB2	2:A:2001:ADP:O2B	2.18	0.44
1:B:1805:LYS:N	1:B:1818:GLN:O	2.40	0.44
1:B:200:ARG:O	1:B:203:GLU:HG2	2.18	0.44
1:B:1810:ASN:ND2	1:B:1836:ILE:HG21	2.33	0.44
1:B:1840:ASP:O	1:B:1843:ILE:HG23	2.18	0.44
1:A:1322:ILE:HG23	1:A:1830:ASP:HB2	1.99	0.44
1:A:1956:MET:O	1:A:1960:LEU:HG	2.18	0.44
1:B:1311:LYS:HZ3	1:B:1317:ARG:CD	2.31	0.44
1:A:237:LEU:HD23	1:A:257:MET:HB2	2.00	0.43
1:A:1894:ILE:HD11	1:A:1925:LEU:CD1	2.47	0.43
1:A:1960:LEU:HA	1:A:1963:ILE:CG1	2.48	0.43
1:A:1346:PRO:HB3	1:A:1872:ARG:HD3	2.00	0.43
1:A:1848:ALA:O	1:A:1849:ARG:C	2.61	0.43
1:B:169:THR:HB	1:B:170:ILE:HD12	2.00	0.43
1:B:215:ILE:HD12	1:B:217:LEU:HD21	1.99	0.43
1:B:1269:ILE:CG2	1:B:1270:LYS:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1815:PRO:HD3	1:B:1965:MET:CE	2.41	0.43
1:B:1868:HIS:O	1:B:1869:GLU:C	2.59	0.43
1:B:1902:ARG:NH1	1:B:1902:ARG:HG2	2.32	0.43
1:A:164:VAL:HG21	1:A:244:PRO:HB2	2.00	0.43
1:A:1266:GLU:O	1:A:1269:ILE:HG23	2.19	0.43
1:B:1899:VAL:HG13	1:B:1900:ARG:N	2.33	0.43
1:A:168:PRO:O	1:A:168:PRO:HG2	2.17	0.43
1:B:233:VAL:HG12	1:B:257:MET:CE	2.48	0.43
1:B:1759:ASP:OD1	1:B:1760:GLU:N	2.51	0.43
1:B:1809:PHE:HB2	1:B:1818:GLN:NE2	2.33	0.43
1:B:1851:ILE:HG12	2:B:2001:ADP:O2'	2.18	0.43
1:A:153:PHE:CD1	1:A:153:PHE:N	2.87	0.43
1:A:1265:GLU:OE2	1:A:1873:LYS:HE3	2.18	0.43
1:B:130:VAL:HG23	1:B:227:PRO:HG3	2.01	0.43
1:B:204:VAL:HG21	1:B:210:PRO:HB3	2.00	0.43
1:B:233:VAL:CG1	1:B:257:MET:HE1	2.49	0.43
1:B:1311:LYS:HG2	1:B:1317:ARG:CB	2.48	0.43
1:B:1919:PRO:CG	1:B:1920:ILE:H	2.29	0.43
1:A:191:ASP:HB3	1:A:222:VAL:HG21	2.00	0.43
1:A:1286:ILE:HD13	1:A:1286:ILE:HA	1.91	0.43
1:A:1308:VAL:O	1:A:1309:SER:HB3	2.19	0.43
1:A:1311:LYS:NZ	1:A:1319:ARG:HA	2.34	0.43
1:A:1353:GLY:O	1:A:1764:MET:HA	2.19	0.43
1:B:1865:LYS:C	1:B:1866:ILE:HD12	2.43	0.43
1:A:138:TYR:OH	1:A:188:LYS:HD2	2.18	0.43
1:A:140:ALA:O	1:A:154:GLU:HA	2.19	0.43
1:A:1290:ILE:HA	2:A:2001:ADP:C2	2.53	0.43
1:B:1300:ILE:O	1:B:1304:LEU:HG	2.18	0.43
1:B:1939:ARG:NH1	1:B:1948:ASP:OD2	2.52	0.43
1:B:121:ILE:HD12	1:B:123:ILE:HD11	1.99	0.43
1:B:1885:VAL:O	1:B:1944:VAL:HG23	2.19	0.43
1:A:1328:GLY:HA3	1:A:1334:LYS:HD2	2.01	0.43
1:B:1811:ARG:HG3	1:B:1813:LYS:HB2	2.01	0.43
1:B:162:PRO:HG2	1:B:166:GLU:OE2	2.18	0.43
1:B:205:PRO:O	1:B:208:GLN:HB2	2.19	0.43
1:B:1308:VAL:O	1:B:1309:SER:HB3	2.18	0.43
1:B:1842:LYS:O	1:B:1845:SER:HB3	2.19	0.43
1:B:1926:GLU:O	1:B:1930:ARG:HG3	2.19	0.43
1:A:105:ARG:NH2	1:A:116:ASP:OD1	2.50	0.42
1:A:1311:LYS:HE3	1:A:1317:ARG:NH2	2.34	0.42
1:A:1939:ARG:NH1	1:A:1948:ASP:CG	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:VAL:HB	1:B:257:MET:HE1	2.00	0.42
1:B:241:GLN:HE21	1:B:241:GLN:HB2	1.50	0.42
1:B:1318:LEU:HD22	1:B:1318:LEU:HA	1.89	0.42
1:A:1939:ARG:HH22	1:A:1945:THR:HG1	1.66	0.42
1:B:1811:ARG:HA	1:B:1812:MET:HE2	2.01	0.42
1:A:1840:ASP:HB3	1:A:1843:ILE:HG12	2.02	0.42
1:A:1860:GLU:HB2	1:A:1862:VAL:HG22	2.00	0.42
1:A:1935:HIS:CE1	1:A:1951:GLU:HG3	2.54	0.42
1:A:204:VAL:HA	1:A:205:PRO:HD3	1.77	0.42
1:A:1762:ASP:OD1	1:A:1820:ASP:HB3	2.20	0.42
1:A:1894:ILE:HG23	1:A:1895:GLU:H	1.83	0.42
1:A:1929:ILE:HD12	1:A:1929:ILE:H	1.84	0.42
1:A:1947:GLU:O	1:A:1951:GLU:HG2	2.19	0.42
1:B:12:ASP:O	1:B:16:GLU:HB2	2.18	0.42
1:B:110:ARG:O	1:B:113:ARG:NH2	2.52	0.42
1:B:245:VAL:HG22	1:B:245:VAL:O	2.19	0.42
1:A:78:LEU:O	1:A:82:ILE:HG13	2.20	0.42
1:A:1733:VAL:HG12	1:A:1734:ARG:N	2.34	0.42
1:A:1828:ARG:NE	1:A:1923:ARG:NH2	2.51	0.42
1:A:1919:PRO:HG2	1:A:1920:ILE:H	1.84	0.42
1:A:1960:LEU:C	1:A:1963:ILE:HG13	2.44	0.42
1:B:11:ARG:HG2	1:B:77:ALA:HB2	2.02	0.42
1:B:143:LYS:HA	1:B:151:GLN:O	2.18	0.42
1:B:241:GLN:HG2	1:B:243:SER:O	2.19	0.42
1:B:1733:VAL:CG1	1:B:1734:ARG:N	2.82	0.42
1:B:1839:PRO:O	1:B:1843:ILE:HG23	2.18	0.42
1:B:1878:ALA:HA	1:B:1882:ILE:CG1	2.47	0.42
1:A:138:TYR:CD1	1:A:138:TYR:C	2.98	0.42
1:B:1296:VAL:HA	1:B:1833:PHE:CE2	2.55	0.42
1:B:1815:PRO:CD	1:B:1965:MET:HE2	2.42	0.42
1:B:1289:ALA:CB	1:B:1340:TYR:HE2	2.32	0.42
1:B:1335:SER:HA	1:B:1759:ASP:OD2	2.20	0.42
1:B:1344:LEU:O	1:B:1346:PRO:HD3	2.20	0.42
1:B:1882:ILE:HG23	1:B:1942:PRO:HB3	2.01	0.42
1:B:1901:MET:HE3	1:B:1920:ILE:HG21	2.01	0.42
1:A:1811:ARG:HH11	1:A:1813:LYS:HD2	1.84	0.42
1:A:1862:VAL:HG23	1:A:1862:VAL:O	2.18	0.42
1:A:1316:THR:HB	1:A:1317:ARG:H	1.62	0.42
1:A:1327:VAL:HG11	1:A:1819:ILE:HG21	2.02	0.42
1:A:1342:ALA:HB2	1:A:1757:LEU:CD1	2.50	0.42
1:A:1811:ARG:HD3	1:A:1813:LYS:CG	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1283:VAL:CG2	1:B:1284:ASP:N	2.83	0.42
1:B:1342:ALA:O	1:B:1345:ALA:CB	2.65	0.42
1:B:1879:ARG:HG2	1:B:1879:ARG:NH1	2.32	0.42
1:A:155:TRP:HA	1:A:155:TRP:HE3	1.83	0.42
1:A:1312:LEU:HB3	1:A:1313:PRO:CD	2.43	0.42
1:A:1815:PRO:CG	1:A:1965:MET:HE2	2.50	0.42
1:A:1839:PRO:HB2	1:B:1903:LYS:HZ3	1.85	0.42
1:A:1899:VAL:CG1	1:A:1900:ARG:N	2.83	0.42
1:B:1814:ASN:ND2	1:B:1817:GLU:OE2	2.53	0.42
1:A:53:LEU:HA	1:A:60:ALA:HB2	2.01	0.41
1:A:1734:ARG:HH11	1:A:1734:ARG:CG	2.33	0.41
1:B:233:VAL:HG12	1:B:257:MET:HE1	2.02	0.41
1:A:25:ASN:N	1:A:27:GLN:HE21	2.07	0.41
1:A:1942:PRO:O	1:A:1942:PRO:HG2	2.20	0.41
1:A:155:TRP:CG	1:A:156:PRO:N	2.88	0.41
1:A:156:PRO:CD	1:A:161:MET:HG2	2.49	0.41
1:A:1884:PRO:HA	1:A:1942:PRO:HB2	2.01	0.41
1:A:1941:SER:CB	1:A:1943:ILE:N	2.84	0.41
1:B:183:ILE:HG22	1:B:186:LYS:H	1.85	0.41
1:A:143:LYS:HB2	1:A:183:ILE:CD1	2.37	0.41
1:A:156:PRO:HD3	1:A:161:MET:HG2	2.02	0.41
1:A:240:LYS:HB3	1:A:256:TYR:CD1	2.56	0.41
1:A:1308:VAL:CG1	1:A:1309:SER:H	2.33	0.41
1:A:1278:ILE:O	1:A:1282:ILE:HG13	2.20	0.41
1:A:1851:ILE:HD12	1:B:1925:LEU:HD23	2.03	0.41
1:A:1928:LEU:HA	1:A:1928:LEU:HD13	1.70	0.41
1:B:82:ILE:CD1	1:B:96:VAL:HG11	2.51	0.41
1:B:1729:THR:O	1:B:1746:GLY:N	2.46	0.41
1:B:1773:HIS:HD2	1:B:1828:ARG:NH1	2.19	0.41
1:B:1869:GLU:HA	1:B:1872:ARG:NH1	2.35	0.41
1:B:1898:TYR:CD1	1:B:1925:LEU:HD13	2.56	0.41
1:A:155:TRP:O	1:A:157:GLU:HG3	2.20	0.41
1:A:1882:ILE:H	1:A:1882:ILE:CD1	2.15	0.41
1:B:30:TYR:O	1:B:34:ILE:HG13	2.21	0.41
1:B:138:TYR:CZ	1:B:188:LYS:HB3	2.55	0.41
1:A:1335:SER:HA	1:A:1759:ASP:OD2	2.21	0.41
1:A:1767:ARG:HH11	1:A:1767:ARG:CG	2.33	0.41
1:B:88:THR:O	1:B:89:TYR:C	2.63	0.41
1:B:1760:GLU:HG2	1:B:1763:LYS:HD2	2.02	0.41
1:B:1880:LYS:O	1:B:1883:HIS:HE1	2.03	0.41
1:A:161:MET:SD	1:A:165:LEU:HD13	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PRO:C	1:A:245:VAL:HG13	2.45	0.41
1:A:1946:ARG:HB3	1:A:1950:ARG:HE	1.86	0.41
1:B:61:TYR:OH	1:B:260:SER:HB3	2.21	0.41
1:B:1262:SER:C	1:B:1264:GLU:N	2.79	0.41
1:B:1287:ALA:O	1:B:1290:ILE:CG1	2.68	0.41
1:B:1944:VAL:HG12	1:B:1948:ASP:HB3	2.01	0.41
1:A:121:ILE:HD12	1:A:123:ILE:HD11	2.03	0.41
1:A:147:PRO:HA	1:A:150:MET:HE2	2.02	0.41
1:A:1281:ALA:O	1:A:1285:SER:N	2.54	0.41
1:A:1772:ILE:HG23	1:A:1773:HIS:N	2.35	0.41
1:A:1811:ARG:O	1:A:1813:LYS:N	2.54	0.41
1:A:1940:LEU:O	1:A:1941:SER:C	2.62	0.41
1:B:1733:VAL:HG12	1:B:1734:ARG:N	2.35	0.41
1:B:1783:ILE:O	1:B:1789:THR:HA	2.21	0.41
1:B:1814:ASN:OD1	1:B:1814:ASN:N	2.54	0.41
1:B:1863:ALA:HB1	1:B:1864:PRO:CD	2.42	0.41
1:B:1868:HIS:O	1:B:1871:LEU:N	2.53	0.41
1:B:1920:ILE:HD13	1:B:1920:ILE:HA	1.87	0.41
1:A:144:HIS:CE1	1:A:174:CYS:SG	3.13	0.41
1:B:142:TYR:HD2	1:B:155:TRP:HB2	1.86	0.41
1:A:142:TYR:CE1	1:A:182:LEU:HB2	2.56	0.40
1:A:1336:GLN:HE21	1:A:1340:TYR:HE1	1.69	0.40
1:A:1344:LEU:O	1:A:1346:PRO:HD3	2.21	0.40
1:A:1761:LEU:HD11	1:A:1764:MET:CE	2.51	0.40
1:B:1311:LYS:HZ3	1:B:1317:ARG:CG	2.34	0.40
1:B:1840:ASP:O	1:B:1841:ASP:C	2.64	0.40
1:B:1875:ILE:HG22	1:B:1879:ARG:HD3	2.03	0.40
1:B:1963:ILE:C	1:B:1965:MET:N	2.77	0.40
1:A:182:LEU:HG	1:A:183:ILE:N	2.34	0.40
1:B:1939:ARG:O	1:B:1940:LEU:HD12	2.20	0.40
1:B:1939:ARG:NH2	1:B:1945:THR:OG1	2.55	0.40
1:A:1361:LEU:HB2	1:A:1768:ASP:OD2	2.20	0.40
1:A:1868:HIS:O	1:A:1869:GLU:C	2.62	0.40
1:A:144:HIS:ND1	1:A:171:CYS:HB2	2.35	0.40
1:A:1843:ILE:HG13	1:A:1844:ASP:H	1.86	0.40
1:B:152:GLU:OE1	1:B:186:LYS:NZ	2.32	0.40
1:B:155:TRP:HB3	1:B:156:PRO:HD2	2.04	0.40
1:A:1950:ARG:HH11	1:A:1950:ARG:CG	2.35	0.40
1:B:69:ILE:O	1:B:72:PRO:HD2	2.22	0.40
1:B:1860:GLU:O	1:B:1861:VAL:C	2.65	0.40
1:B:1899:VAL:CG1	1:B:1900:ARG:N	2.84	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	A	587/613 (96%)	519 (88%)	53 (9%)	15 (3%)	4	11
1	B	587/613 (96%)	524 (89%)	47 (8%)	16 (3%)	4	10
All	All	1174/1226 (96%)	1043 (89%)	100 (8%)	31 (3%)	4	11

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	TRP
1	A	247	ARG
1	A	1841	ASP
1	A	1857	GLY
1	B	155	TRP
1	B	245	VAL
1	B	1841	ASP
1	B	1861	VAL
1	B	1948	ASP
1	A	245	VAL
1	A	1812	MET
1	A	1858	GLU
1	B	1289	ALA
1	B	1811	ARG
1	B	1839	PRO
1	A	139	LYS
1	A	156	PRO
1	A	1289	ALA
1	A	1868	HIS
1	B	156	PRO
1	B	1346	PRO
1	B	1859	SER

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Mol	Chain	Res	Type
1	A	250	ARG
1	A	1346	PRO
1	B	1309	SER
1	B	1854	VAL
1	B	89	TYR
1	A	168	PRO
1	B	1941	SER
1	A	1942	PRO
1	B	1942	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	A	517/537 (96%)	433 (84%)	84 (16%)	2	6
1	B	517/537 (96%)	445 (86%)	72 (14%)	3	9
All	All	1034/1074 (96%)	878 (85%)	156 (15%)	3	7

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	13	VAL
1	A	27	GLN
1	A	46	ILE
1	A	48	GLU
1	A	71	LEU
1	A	91	ARG
1	A	113	ARG
1	A	127	LEU
1	A	139	LYS
1	A	161	MET
1	A	163	GLU
1	A	165	LEU
1	A	167	MET

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Mol	Chain	Res	Type
1	A	168	PRO
1	A	169	THR
1	A	181	ARG
1	A	182	LEU
1	A	188	LYS
1	A	197	ILE
1	A	202	GLU
1	A	222	VAL
1	A	233	VAL
1	A	241	GLN
1	A	245	VAL
1	A	247	ARG
1	A	264	VAL
1	A	265	SER
1	A	269	LEU
1	A	1267	GLN
1	A	1269	ILE
1	A	1276	LYS
1	A	1283	VAL
1	A	1285	SER
1	A	1286	ILE
1	A	1308	VAL
1	A	1311	LYS
1	A	1316	THR
1	A	1318	LEU
1	A	1347	ARG
1	A	1352	SER
1	A	1355	SER
1	A	1734	ARG
1	A	1760	GLU
1	A	1762	ASP
1	A	1763	LYS
1	A	1764	MET
1	A	1766	ASP
1	A	1770	SER
1	A	1779	GLN
1	A	1788	ILE
1	A	1805	LYS
1	A	1806	GLN
1	A	1808	ARG
1	A	1809	PHE
1	A	1818	GLN

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Mol	Chain	Res	Type
1	A	1825	LEU
1	A	1841	ASP
1	A	1843	ILE
1	A	1855	ARG
1	A	1858	GLU
1	A	1861	VAL
1	A	1869	GLU
1	A	1882	ILE
1	A	1886	ILE
1	A	1888	GLU
1	A	1892	GLU
1	A	1894	ILE
1	A	1895	GLU
1	A	1896	LYS
1	A	1901	MET
1	A	1903	LYS
1	A	1921	THR
1	A	1928	LEU
1	A	1939	ARG
1	A	1940	LEU
1	A	1941	SER
1	A	1942	PRO
1	A	1943	ILE
1	A	1944	VAL
1	A	1950	ARG
1	A	1953	ILE
1	A	1961	LYS
1	A	1963	ILE
1	B	8	ILE
1	B	9	ASP
1	B	13	VAL
1	B	27	GLN
1	B	48	GLU
1	B	68	LYS
1	B	88	THR
1	B	91	ARG
1	B	93	ILE
1	B	96	VAL
1	B	103	ILE
1	B	113	ARG
1	B	127	LEU
1	B	139	LYS

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Mol	Chain	Res	Type
1	B	141	THR
1	B	143	LYS
1	B	158	ASP
1	B	161	MET
1	B	163	GLU
1	B	166	GLU
1	B	169	THR
1	B	202	GLU
1	B	222	VAL
1	B	233	VAL
1	B	241	GLN
1	B	247	ARG
1	B	254	ASP
1	B	264	VAL
1	B	1261	ILE
1	B	1269	ILE
1	B	1272	LEU
1	B	1276	LYS
1	B	1314	ASP
1	B	1316	THR
1	B	1318	LEU
1	B	1329	ASP
1	B	1334	LYS
1	B	1347	ARG
1	B	1762	ASP
1	B	1766	ASP
1	B	1770	SER
1	B	1796	THR
1	B	1808	ARG
1	B	1809	PHE
1	B	1812	MET
1	B	1813	LYS
1	B	1814	ASN
1	B	1824	THR
1	B	1825	LEU
1	B	1842	LYS
1	B	1843	ILE
1	B	1846	GLU
1	B	1850	HIS
1	B	1860	GLU
1	B	1862	VAL
1	B	1869	GLU

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Mol	Chain	Res	Type
1	B	1873	LYS
1	B	1879	ARG
1	B	1885	VAL
1	B	1886	ILE
1	B	1891	MET
1	B	1892	GLU
1	B	1896	LYS
1	B	1900	ARG
1	B	1902	ARG
1	B	1921	THR
1	B	1939	ARG
1	B	1941	SER
1	B	1944	VAL
1	B	1948	ASP
1	B	1950	ARG
1	B	1953	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	27	GLN
1	A	1267	GLN
1	A	1336	GLN
1	A	1779	GLN
1	A	1883	HIS
1	A	1962	GLN
1	B	27	GLN
1	B	97	HIS
1	B	241	GLN
1	B	1336	GLN
1	B	1779	GLN
1	B	1810	ASN
1	B	1850	HIS
1	B	1962	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 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADP	B	2001	3	28,29,29	1.40	4 (14%)	43,45,45	1.88	8 (18%)
2	ADP	A	2001	3	28,29,29	1.28	3 (10%)	43,45,45	1.80	10 (23%)

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	2001	3	-	2/16/32/32	0/3/3/3
2	ADP	A	2001	3	-	2/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	ADP	PB-O1B	3.45	1.61	1.50
2	A	2001	ADP	PB-O1B	3.27	1.60	1.50
2	B	2001	ADP	PA-O3A	2.69	1.62	1.59
2	A	2001	ADP	PA-O3A	2.57	1.62	1.59
2	B	2001	ADP	C6-N6	2.26	1.40	1.34
2	B	2001	ADP	C5-C4	2.24	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	ADP	C5-N7	-2.20	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	ADP	C5-C4-N3	-5.99	118.47	126.72
2	A	2001	ADP	C5-C4-N3	-5.20	119.56	126.72
2	B	2001	ADP	N3-C4-N9	5.12	135.87	127.17
2	A	2001	ADP	N3-C2-N1	-4.69	121.48	128.58
2	A	2001	ADP	N3-C4-N9	4.55	134.90	127.17
2	B	2001	ADP	N3-C2-N1	-4.20	122.22	128.58
2	B	2001	ADP	C2-N3-C4	3.86	121.27	111.83
2	A	2001	ADP	C2-N3-C4	3.69	120.83	111.83
2	A	2001	ADP	C5-N7-C8	3.66	109.21	103.45
2	B	2001	ADP	C5-N7-C8	3.61	109.12	103.45
2	B	2001	ADP	C4-C5-N7	-2.68	107.52	110.58
2	A	2001	ADP	C4-C5-N7	-2.40	107.84	110.58
2	A	2001	ADP	PA-O5'-C5'	-2.29	108.23	121.35
2	B	2001	ADP	PA-O5'-C5'	-2.22	108.62	121.35
2	B	2001	ADP	C3'-C2'-C1'	2.12	105.48	101.46
2	A	2001	ADP	C2-N1-C6	2.06	122.11	118.73
2	A	2001	ADP	C3'-C2'-C1'	2.02	105.28	101.46
2	A	2001	ADP	N9-C8-N7	-2.02	111.08	113.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2001	ADP	C2'-C1'-N9-C4
2	A	2001	ADP	C2'-C1'-N9-C8
2	A	2001	ADP	C2'-C1'-N9-C4
2	B	2001	ADP	C2'-C1'-N9-C8

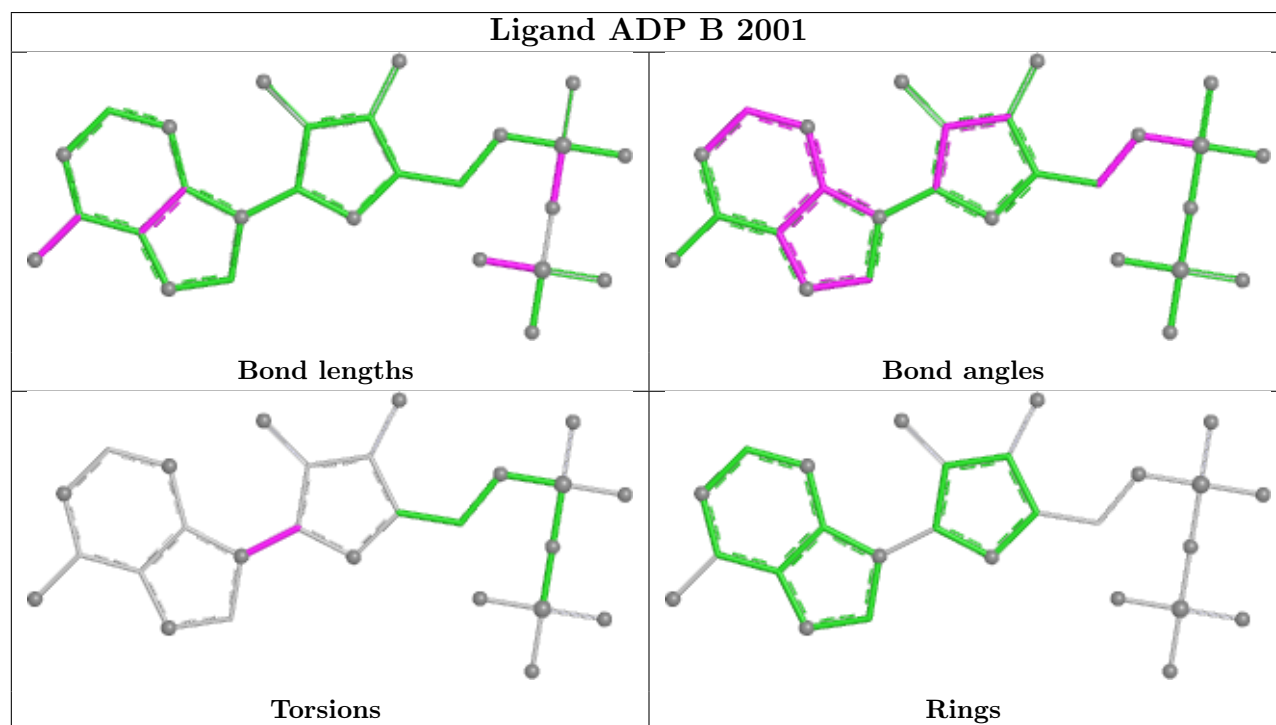
There are no ring outliers.

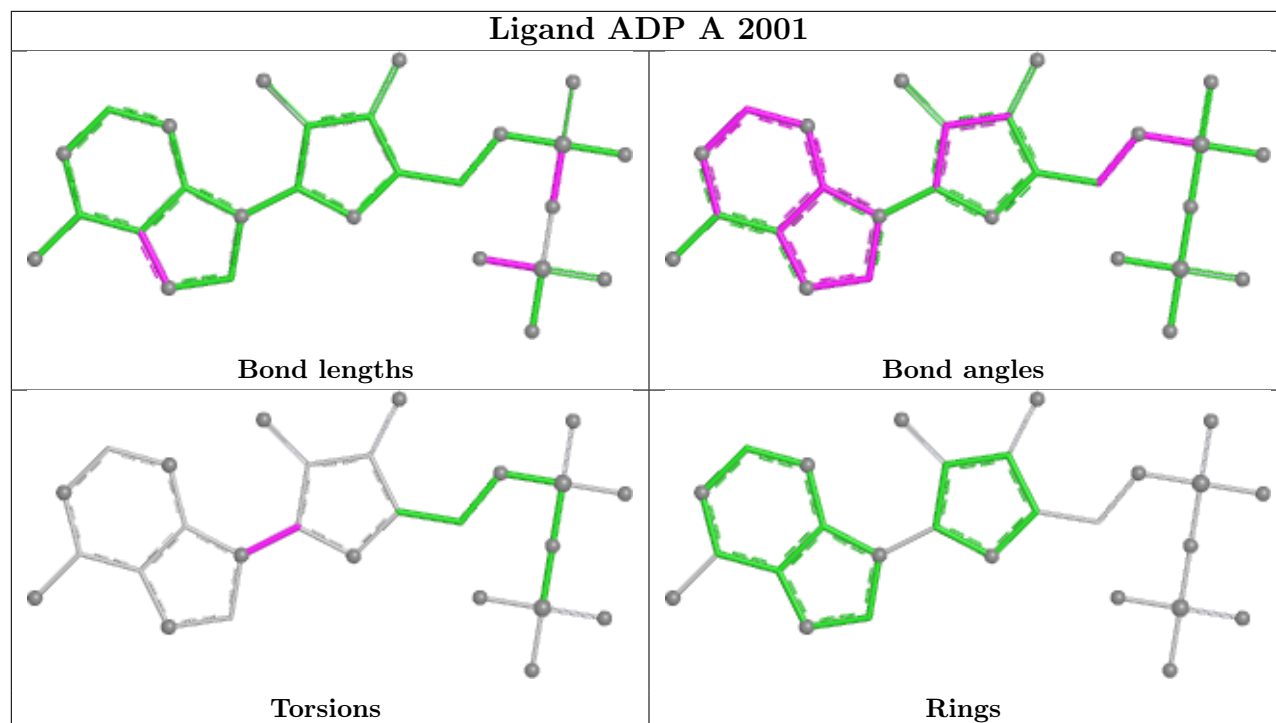
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	ADP	1	0
2	A	2001	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	A	591/613 (96%)	0.79	113 (19%)	3 3	10, 63, 109, 125	0
1	B	591/613 (96%)	0.80	104 (17%)	4 3	9, 61, 110, 128	0
All	All	1182/1226 (96%)	0.79	217 (18%)	3 3	9, 62, 110, 128	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1315	GLY	6.9
1	B	249	SER	5.5
1	A	1862	VAL	5.5
1	B	1862	VAL	4.9
1	B	248	GLY	4.8
1	B	177	PRO	4.7
1	A	1315	GLY	4.3
1	A	155	TRP	4.2
1	B	1346	PRO	4.2
1	A	1312	LEU	4.2
1	B	1949	ALA	4.2
1	A	165	LEU	4.1
1	A	249	SER	4.1
1	A	1346	PRO	4.0
1	A	1861	VAL	4.0
1	B	1854	VAL	4.0
1	B	1316	THR	3.9
1	A	177	PRO	3.9
1	B	147	PRO	3.9
1	A	1810	ASN	3.8
1	A	1316	THR	3.8
1	B	146	HIS	3.8
1	A	173	LYS	3.8
1	B	1291	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	164	VAL	3.7
1	B	8	ILE	3.7
1	A	175	GLY	3.6
1	B	1807	GLY	3.6
1	B	1901	MET	3.6
1	B	1941	SER	3.6
1	B	170	ILE	3.6
1	B	1886	ILE	3.6
1	A	159	GLU	3.6
1	B	1942	PRO	3.5
1	B	1317	ARG	3.5
1	A	1261	ILE	3.5
1	A	1866	ILE	3.5
1	B	1948	ASP	3.5
1	A	8	ILE	3.5
1	A	1855	ARG	3.5
1	B	148	ASP	3.4
1	A	1279	VAL	3.4
1	A	150	MET	3.4
1	B	150	MET	3.4
1	B	1859	SER	3.4
1	B	1312	LEU	3.4
1	A	147	PRO	3.4
1	A	1272	LEU	3.4
1	A	1939	ARG	3.4
1	A	1886	ILE	3.3
1	A	1291	TYR	3.3
1	B	154	GLU	3.3
1	A	1854	VAL	3.3
1	B	178	GLY	3.3
1	A	1901	MET	3.3
1	B	1861	VAL	3.3
1	B	1851	ILE	3.3
1	B	1272	LEU	3.2
1	B	1852	LEU	3.2
1	B	181	ARG	3.2
1	B	169	THR	3.2
1	A	1859	SER	3.2
1	B	1353	GLY	3.2
1	B	1863	ALA	3.2
1	A	178	GLY	3.2
1	A	1278	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	160	GLU	3.1
1	B	145	ILE	3.1
1	B	1310	ARG	3.1
1	A	1259	LEU	3.1
1	A	154	GLU	3.1
1	B	159	GLU	3.1
1	A	169	THR	3.1
1	B	1338	LEU	3.1
1	A	1942	PRO	3.1
1	B	1331	GLY	3.1
1	B	7	GLN	3.0
1	A	1885	VAL	3.0
1	B	1261	ILE	3.0
1	B	1313	PRO	3.0
1	B	1919	PRO	3.0
1	B	1939	ARG	3.0
1	A	146	HIS	2.9
1	B	1904	SER	2.9
1	B	1345	ALA	2.9
1	A	1940	LEU	2.9
1	A	176	LYS	2.9
1	A	1843	ILE	2.9
1	A	1340	TYR	2.9
1	A	152	GLU	2.8
1	A	170	ILE	2.8
1	A	1851	ILE	2.8
1	A	153	PHE	2.8
1	A	1313	PRO	2.8
1	A	246	LYS	2.8
1	A	1350	TYR	2.8
1	A	1310	ARG	2.8
1	A	1311	LYS	2.8
1	A	1891	MET	2.8
1	A	157	GLU	2.8
1	B	1287	ALA	2.8
1	B	1890	ALA	2.8
1	A	1314	ASP	2.7
1	B	1855	ARG	2.7
1	B	1340	TYR	2.7
1	A	1867	PRO	2.7
1	A	1344	LEU	2.7
1	A	248	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1856	ARG	2.7
1	B	1887	SER	2.7
1	B	246	LYS	2.7
1	A	145	ILE	2.7
1	A	172	PRO	2.7
1	B	1263	PRO	2.7
1	B	247	ARG	2.6
1	A	1289	ALA	2.6
1	A	143	LYS	2.6
1	A	1270	LYS	2.6
1	A	1308	VAL	2.6
1	B	155	TRP	2.6
1	A	1938	MET	2.6
1	A	1809	PHE	2.6
1	A	1922	ALA	2.6
1	A	1943	ILE	2.6
1	A	1852	LEU	2.6
1	B	250	ARG	2.6
1	B	1898	TYR	2.6
1	B	1850	HIS	2.6
1	A	166	GLU	2.6
1	A	247	ARG	2.5
1	B	1839	PRO	2.5
1	B	1350	TYR	2.5
1	A	1353	GLY	2.5
1	A	1816	PHE	2.5
1	A	1290	ILE	2.5
1	B	1864	PRO	2.5
1	B	1279	VAL	2.5
1	A	180	PHE	2.5
1	B	1809	PHE	2.5
1	A	1268	ILE	2.5
1	A	1263	PRO	2.5
1	B	156	PRO	2.5
1	B	184	PRO	2.5
1	B	1347	ARG	2.4
1	A	1941	SER	2.4
1	A	138	TYR	2.4
1	A	245	VAL	2.4
1	B	1899	VAL	2.4
1	A	1850	HIS	2.4
1	A	161	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1964	ALA	2.4
1	B	1344	LEU	2.4
1	A	1345	ALA	2.4
1	B	153	PHE	2.4
1	A	1338	LEU	2.3
1	B	241	GLN	2.3
1	A	1899	VAL	2.3
1	B	245	VAL	2.3
1	B	1348	ALA	2.3
1	B	1870	ILE	2.3
1	A	1865	LYS	2.3
1	B	1965	MET	2.3
1	A	1884	PRO	2.3
1	B	172	PRO	2.3
1	A	140	ALA	2.3
1	A	1870	ILE	2.3
1	B	1268	ILE	2.3
1	B	1866	ILE	2.3
1	B	1888	GLU	2.3
1	B	1328	GLY	2.3
1	A	1758	ILE	2.2
1	B	1289	ALA	2.2
1	A	156	PRO	2.2
1	A	1919	PRO	2.2
1	A	1807	GLY	2.2
1	B	183	ILE	2.2
1	B	1311	LYS	2.2
1	B	1810	ASN	2.2
1	A	148	ASP	2.2
1	B	1857	GLY	2.2
1	B	1843	ILE	2.2
1	B	1962	GLN	2.2
1	A	1292	GLY	2.2
1	B	1836	ILE	2.2
1	B	1849	ARG	2.2
1	B	1259	LEU	2.2
1	A	1269	ILE	2.2
1	A	1963	ILE	2.2
1	A	167	MET	2.1
1	B	165	LEU	2.1
1	B	160	GLU	2.1
1	A	1961	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	142	TYR	2.1
1	A	1897	TYR	2.1
1	B	1837	ASP	2.1
1	A	243	SER	2.1
1	A	1949	ALA	2.1
1	B	157	GLU	2.1
1	A	1317	ARG	2.1
1	B	179	GLN	2.1
1	B	1812	MET	2.1
1	B	164	VAL	2.1
1	B	1278	ILE	2.1
1	A	1348	ALA	2.1
1	A	1864	PRO	2.1
1	B	1867	PRO	2.1
1	B	1277	ASP	2.0
1	B	1853	ARG	2.0
1	A	162	PRO	2.0
1	A	1965	MET	2.0
1	A	1318	LEU	2.0
1	A	1337	ILE	2.0
1	B	1293	TYR	2.0
1	A	181	ARG	2.0
1	A	250	ARG	2.0
1	A	1863	ALA	2.0
1	B	1286	ILE	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 ⓘ

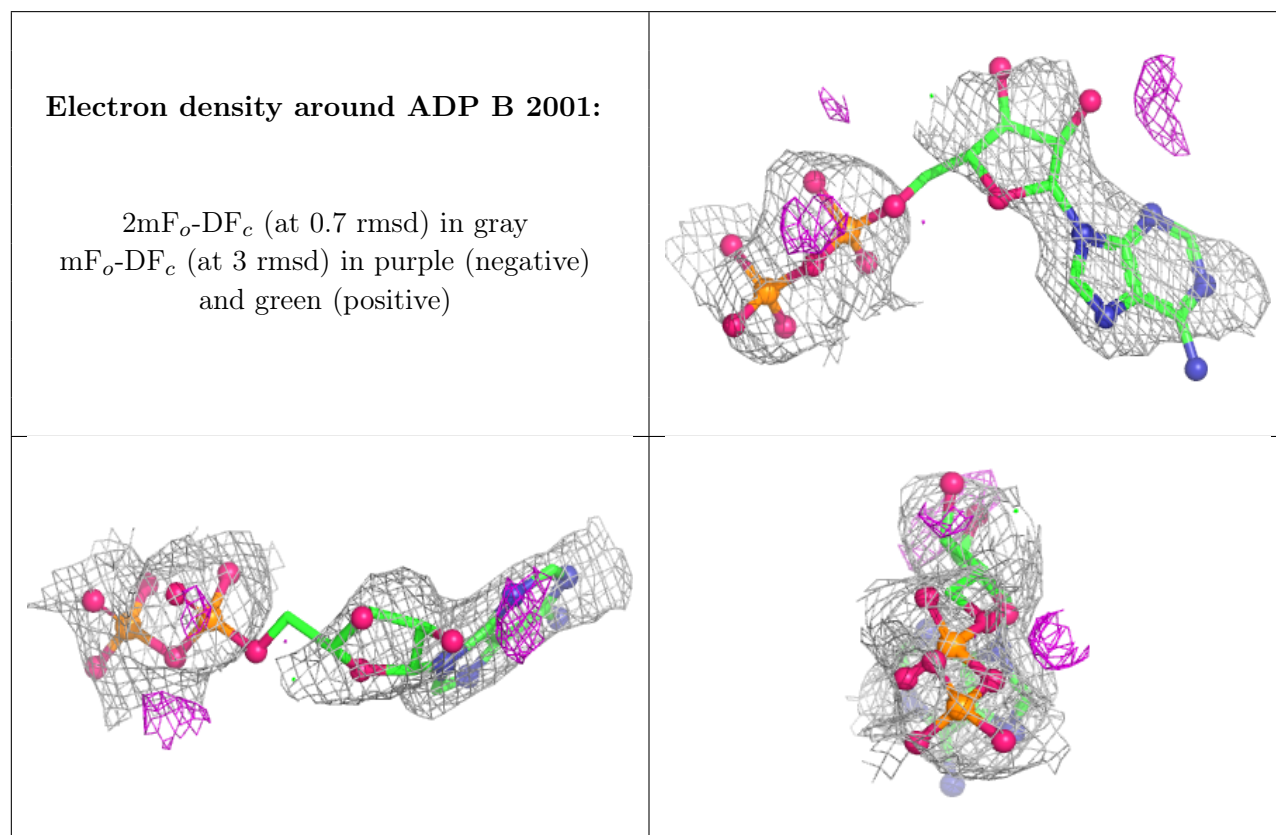
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

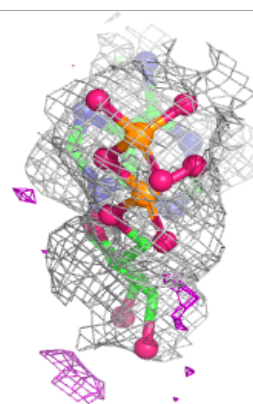
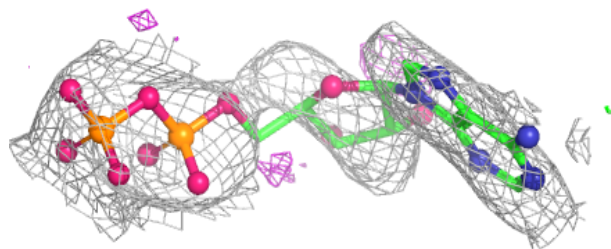
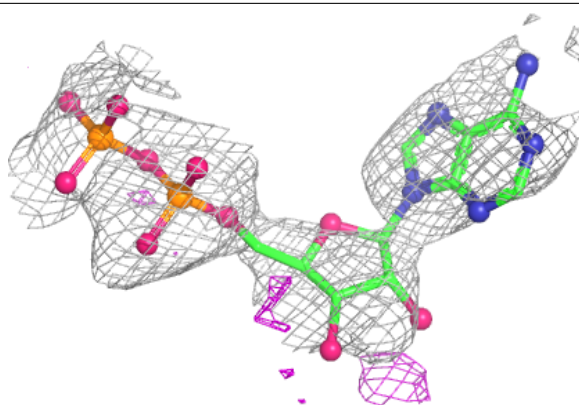
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	B	2001	27/27	0.71	0.20	118,121,127,128	0
2	ADP	A	2001	27/27	0.75	0.19	113,114,115,115	0
3	MG	A	2002	1/1	0.84	0.09	64,64,64,64	0
3	MG	B	2002	1/1	0.86	0.14	64,64,64,64	0
5	CL	A	2005	1/1	0.88	0.10	59,59,59,59	0
4	ZN	B	2003	1/1	0.92	0.07	169,169,169,169	0
4	ZN	A	2003	1/1	0.93	0.07	163,163,163,163	0
5	CL	B	2004	1/1	0.93	0.10	48,48,48,48	0
5	CL	A	2006	1/1	0.94	0.17	41,41,41,41	0
5	CL	B	2005	1/1	0.94	0.06	53,53,53,53	0
5	CL	B	2006	1/1	0.94	0.10	39,39,39,39	0
5	CL	A	2004	1/1	0.96	0.09	48,48,48,48	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 A 2001:

$2mF_o-DF_c$ (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.