Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:29 pm BST

PDB ID	:	1NNE
Title	:	Crystal Structure of the MutS-ADPBeF3-DNA complex
Authors	:	Alani, E.; Lee, J.Y.; Schofield, M.J.; Kijas, A.W.; Hsieh, P.; Yang, W.
Deposited on	:	2003-01-13
Resolution	:	3.11 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:

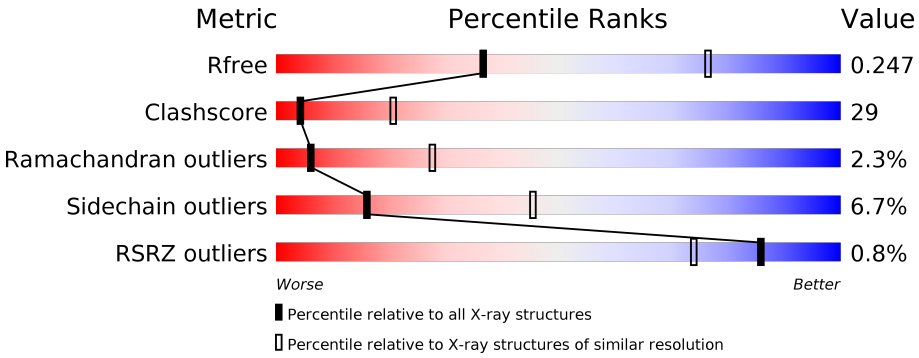
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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 <=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	C	23	9% 9% 83%
2	D	22	14% 14% 82% 5%
3	A	765	52% 43%
3	B	765	% 51% 42% 6%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13089 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 DNA chain called 5'-D(*GP*CP*GP*AP*CP*GP*CP*TP*AP*GP*CP*GP*TP*GP*CP*GP*GP*CP*TP*CP*GP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	23	Total	C	N	O	P	0	0	0
			469	222	87	138	22			

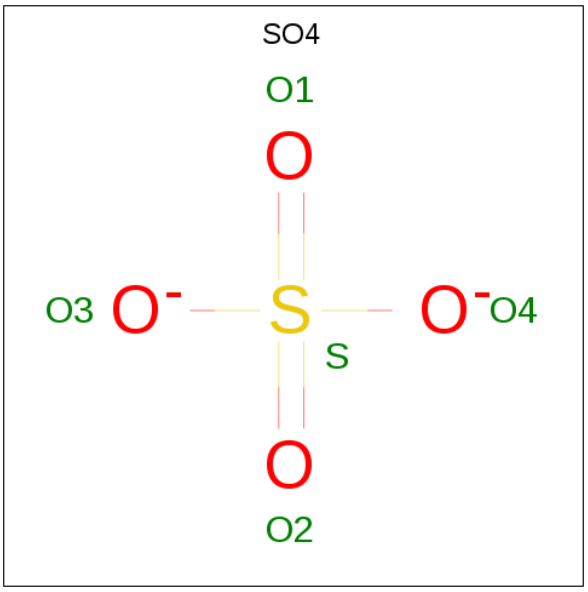
- Molecule 2 is a DNA chain called 5'-D(P*GP*GP*AP*CP*GP*AP*GP*CP*CP*GP*CP*CP*GP*CP*TP*AP*GP*CP*GP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	22	Total	C	N	O	P	0	0	0
			453	212	88	131	22			

- Molecule 3 is a protein called DNA Mismatch Repair protein MutS.

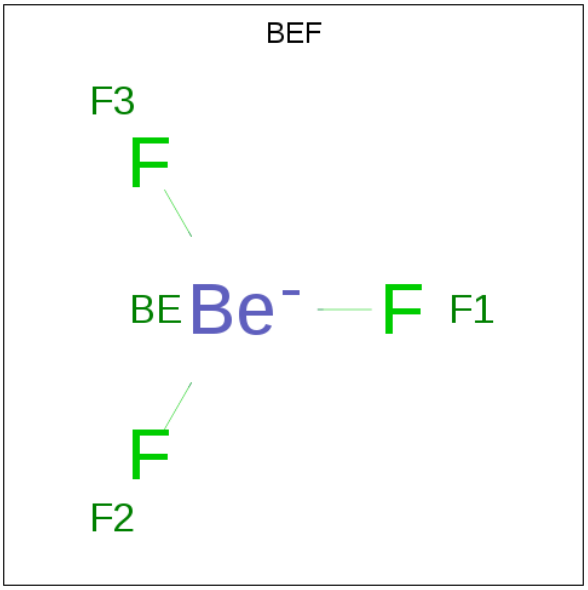
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	759	Total	C	N	O	S	0	0	0
			6006	3825	1068	1099	14			
3	B	759	Total	C	N	O	S	0	0	0
			5986	3813	1065	1094	14			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



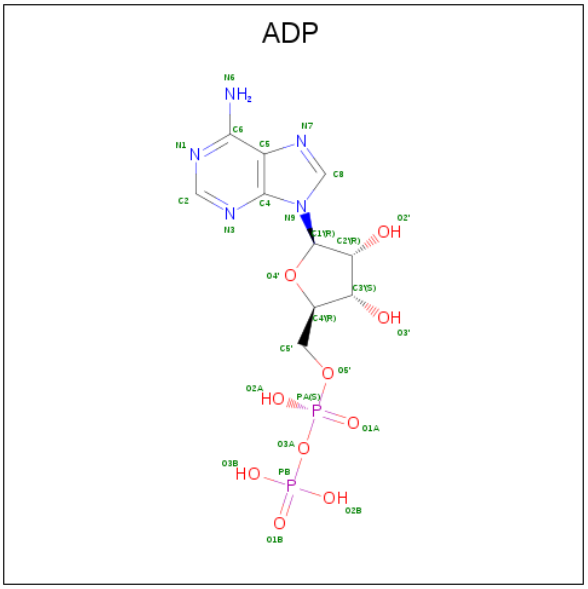
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



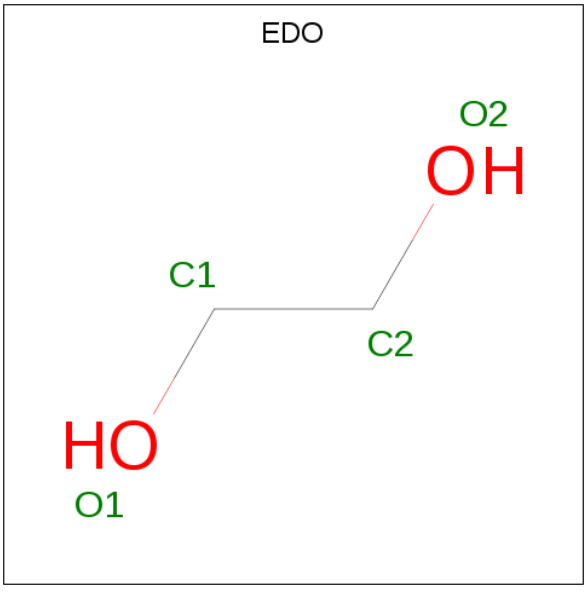
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Be F 4 1 3	0	0
5	B	1	Total Be F 4 1 3	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0

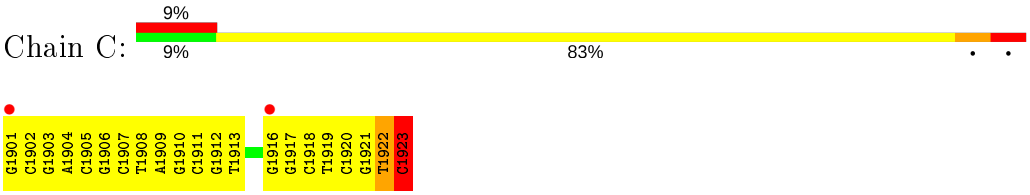
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O 1 1	0	0
8	D	1	Total O 1 1	0	0
8	A	45	Total O 45 45	0	0
8	B	52	Total O 52 52	0	0

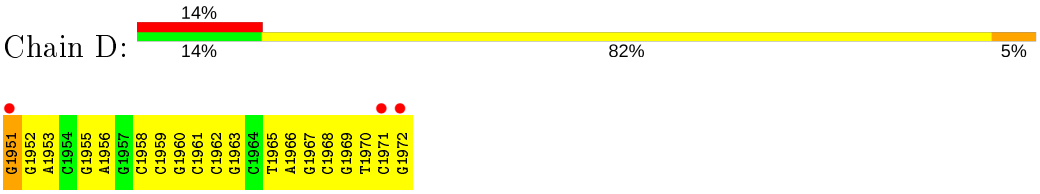
3 Residue-property plots (i)

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.

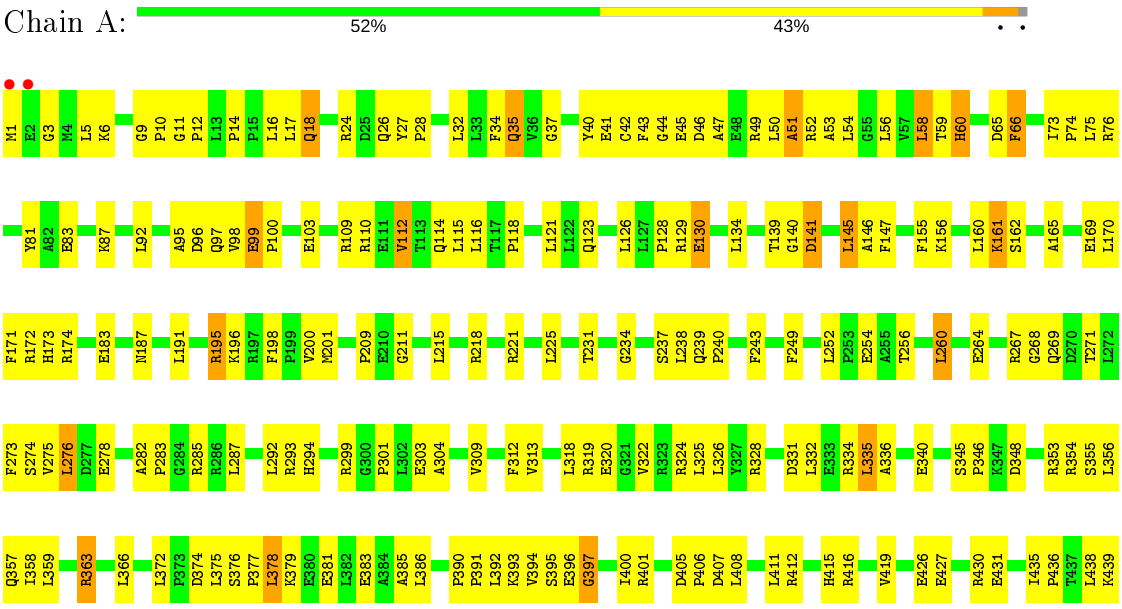
• Molecule 1: 5'-D(*GP*CP*GP*AP*CP*GP*CP*TP*AP*GP*CP*GP*TP*GP*CP*GP*GP*CP*TP*CP*GP*TP*C)-3'

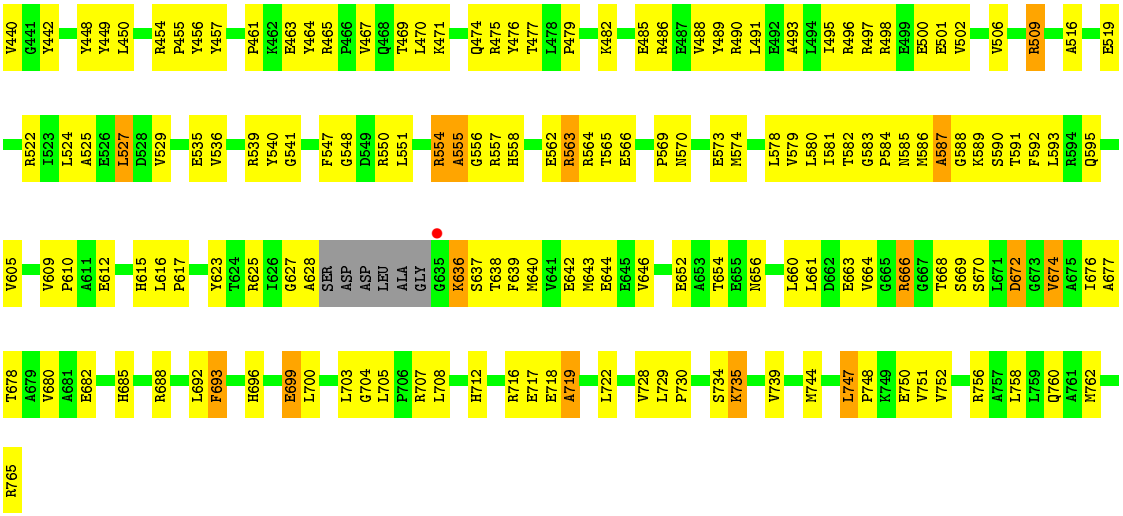


• Molecule 2: 5'-D(P*GP*GP*AP*CP*GP*AP*GP*CP*CP*GP*CP*CP*GP*CP*TP*AP*GP*CP*GP*TP*CP*G)-3'



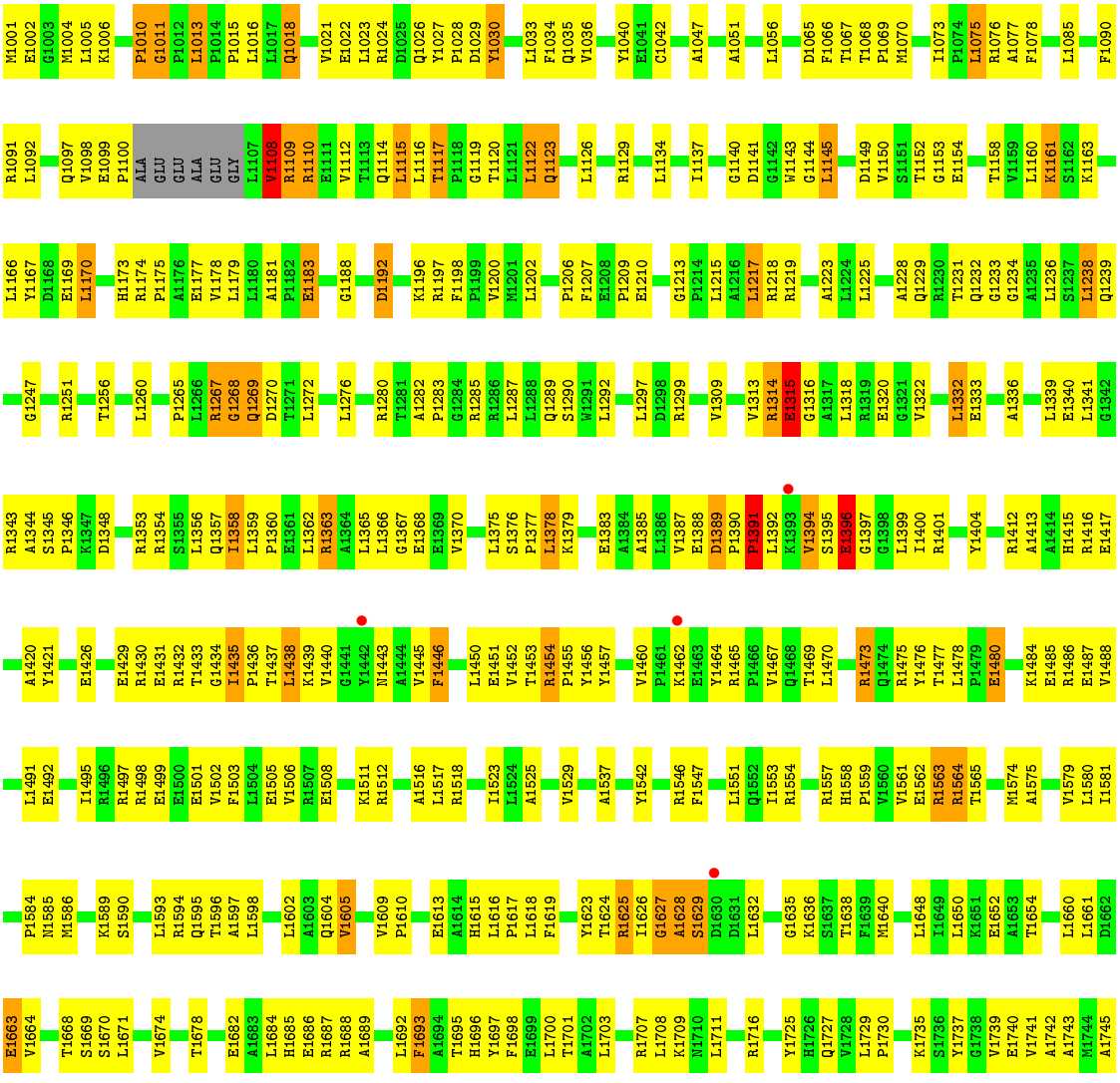
• Molecule 3: DNA Mismatch Repair protein MutS





• Molecule 3: DNA Mismatch Repair protein MutS

Chain B:




G1746
L1747
P1748
V1751
L1758
L1759
Q1760
A1761
M1762
A1763
A1764
R1765

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.44Å 113.22Å 160.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.11 19.94 – 3.11	Depositor EDS
% Data completeness (in resolution range)	87.1 (19.94-3.11) 87.2 (19.94-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.09Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.259 0.199 , 0.247	Depositor DCC
R_{free} test set	1580 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13089	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BEF, SO4, ADP, EDO

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	C	0.87	3/525 (0.6%)	1.59	9/809 (1.1%)
2	D	0.70	2/508 (0.4%)	1.74	11/782 (1.4%)
3	A	0.45	2/6123 (0.0%)	0.72	5/8285 (0.1%)
3	B	0.43	0/6103	0.73	7/8259 (0.1%)
All	All	0.48	7/13259 (0.1%)	0.85	32/18135 (0.2%)

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	C	0	1
3	A	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1923	DC	P-OP1	11.27	1.68	1.49
1	C	1923	DC	P-OP2	-8.57	1.34	1.49
2	D	1951	DG	C2-N3	-7.55	1.26	1.32
1	C	1923	DC	P-O5'	7.50	1.67	1.59
2	D	1951	DG	N9-C4	-6.88	1.32	1.38
3	A	555	ALA	CA-CB	6.67	1.66	1.52
3	A	587	ALA	C-O	-5.08	1.13	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1951	DG	O5'-P-OP1	-25.23	80.42	110.70
1	C	1923	DC	O5'-P-OP1	-22.73	83.42	110.70
2	D	1951	DG	P-O3'-C3'	21.55	145.56	119.70
1	C	1922	DT	O3'-P-O5'	19.06	140.22	104.00
1	C	1923	DC	O5'-P-OP2	-17.75	89.40	110.70
2	D	1951	DG	O3'-P-O5'	15.29	133.04	104.00
2	D	1951	DG	OP1-P-O3'	-13.40	75.73	105.20
3	B	1108	VAL	N-CA-C	-12.86	76.27	111.00
2	D	1951	DG	O5'-P-OP2	-12.72	94.25	105.70
1	C	1922	DT	OP2-P-O3'	9.93	127.05	105.20
1	C	1923	DC	OP1-P-OP2	-9.44	105.44	119.60
1	C	1923	DC	O5'-C5'-C4'	8.55	132.37	111.00
3	A	588	GLY	C-N-CA	8.19	142.19	121.70
3	A	588	GLY	N-CA-C	7.99	133.07	113.10
2	D	1951	DG	O4'-C4'-C3'	-7.06	101.67	104.50
1	C	1922	DT	P-O3'-C3'	6.91	127.99	119.70
2	D	1951	DG	C4-N9-C1'	-6.32	118.28	126.50
3	B	1632	LEU	N-CA-C	-6.25	94.13	111.00
3	A	134	LEU	N-CA-C	-6.01	94.78	111.00
3	B	1268	GLY	N-CA-C	-5.91	98.33	113.10
3	A	555	ALA	N-CA-CB	-5.80	101.99	110.10
3	B	1108	VAL	N-CA-CB	5.75	124.14	111.50
2	D	1951	DG	OP1-P-OP2	5.69	128.14	119.60
3	A	558	HIS	N-CA-C	-5.61	95.86	111.00
2	D	1951	DG	O4'-C1'-N9	-5.55	104.12	108.00
2	D	1951	DG	C8-N9-C1'	5.47	134.11	127.00
3	B	1627	GLY	N-CA-C	5.46	126.74	113.10
1	C	1923	DC	C3'-C2'-C1'	-5.41	96.01	102.50
3	B	1141	ASP	N-CA-CB	5.33	120.19	110.60
2	D	1951	DG	N3-C2-N2	-5.30	116.19	119.90
3	B	1625	ARG	N-CA-C	-5.29	96.73	111.00
1	C	1923	DC	C4'-C3'-C2'	-5.02	98.58	103.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	554	ARG	Mainchain
1	C	1923	DC	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	469	0	259	37	0
2	D	453	0	245	44	1
3	A	6006	0	6093	321	1
3	B	5986	0	6055	371	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
5	A	4	0	0	0	0
5	B	4	0	0	1	0
6	A	27	0	10	0	0
6	B	27	0	10	0	0
7	B	4	0	6	0	0
8	A	45	0	0	1	0
8	B	52	0	0	7	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
All	All	13089	0	12678	750	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (750) 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)
3:A:6:LYS:HD2	3:A:45:GLU:HG2	1.20	1.12
1:C:1916:DG:H2"	1:C:1917:DG:H5'	1.38	1.05
3:B:1597:ALA:HB2	3:B:1660:LEU:HD11	1.38	1.03
3:A:722:LEU:H	3:A:744:MET:HE1	1.24	1.01
1:C:1909:DA:H5"	3:B:1453:THR:HB	1.38	1.00
3:A:6:LYS:HD2	3:A:45:GLU:CG	1.92	0.97
3:A:59:THR:HG22	3:A:60:HIS:H	1.28	0.97
3:A:267:ARG:O	3:A:269:GLN:HG3	1.66	0.95
3:A:557:ARG:NH2	3:A:610:PRO:HA	1.82	0.95
3:A:6:LYS:CD	3:A:45:GLU:HG2	1.95	0.94
3:B:1117:THR:HG23	3:B:1177:GLU:OE1	1.67	0.94
3:A:519:GLU:HG3	3:A:522:ARG:HH11	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1967:DG:H2"	2:D:1968:DC:H5"	1.51	0.90
2:D:1958:DC:H4'	3:B:1443:ASN:HD21	1.36	0.89
2:D:1951:DG:O4'	2:D:1951:DG:N3	2.03	0.89
3:B:1018:GLN:O	3:B:1022:GLU:HG3	1.78	0.84
3:A:35:GLN:HG3	3:A:97:GLN:HG3	1.60	0.83
3:B:1229:GLN:HG2	3:B:1236:LEU:HG	1.60	0.82
3:A:322:VAL:HG11	3:A:527:LEU:HD22	1.59	0.82
3:A:674:VAL:CG1	3:A:699:GLU:HG3	2.10	0.82
3:B:1397:GLY:HA2	3:B:1499:GLU:OE1	1.78	0.82
3:A:677:ALA:HB1	3:A:700:LEU:HD11	1.60	0.81
3:B:1085:LEU:O	3:B:1090:PHE:HB2	1.80	0.81
3:A:557:ARG:HD2	3:A:562:GLU:OE2	1.81	0.80
3:A:722:LEU:H	3:A:744:MET:CE	1.95	0.80
3:B:1318:LEU:HD12	3:B:1365:LEU:HD22	1.64	0.79
3:B:1316:GLY:O	3:B:1320:GLU:HG3	1.82	0.79
3:B:1108:VAL:HG12	3:B:1109:ARG:H	1.46	0.79
1:C:1903:DG:H2"	1:C:1904:DA:C5'	2.12	0.79
1:C:1909:DA:H2"	1:C:1910:DG:H5'	1.65	0.79
3:B:1269:GLN:NE2	3:B:1270:ASP:H	1.80	0.79
3:A:318:LEU:HD11	3:A:366:LEU:HD23	1.65	0.79
3:A:497:ARG:O	3:A:501:GLU:HG3	1.82	0.78
3:B:1379:LYS:O	3:B:1383:GLU:HG3	1.84	0.78
1:C:1921:DG:OP1	3:A:471:LYS:HE3	1.81	0.78
3:A:256:THR:O	3:A:260:LEU:HB2	1.84	0.77
3:A:174:ARG:HH21	3:A:264:GLU:HG2	1.49	0.77
3:B:1034:PHE:CZ	3:B:1110:ARG:HD2	2.19	0.77
3:B:1026:GLN:NE2	8:B:73:HOH:O	2.17	0.77
3:B:1629:SER:CB	3:B:1638:THR:HG23	2.15	0.77
1:C:1909:DA:H5"	3:B:1453:THR:CB	2.14	0.77
3:A:589:LYS:O	3:A:592:PHE:HB3	1.85	0.76
3:B:1160:LEU:HD22	3:B:1166:LEU:HA	1.68	0.76
3:A:672:ASP:O	3:A:676:ILE:HG12	1.86	0.76
3:B:1553:ILE:HD11	3:B:1616:LEU:HD21	1.67	0.76
3:A:490:ARG:HH11	3:A:490:ARG:HG2	1.49	0.76
3:A:519:GLU:HG3	3:A:522:ARG:NH1	2.01	0.76
3:A:35:GLN:HB3	3:A:95:ALA:O	1.86	0.76
1:C:1903:DG:H2"	1:C:1904:DA:H5'	1.67	0.75
3:A:328:ARG:O	3:A:354:ARG:NH1	2.20	0.75
3:A:394:VAL:HG21	3:A:500:GLU:HA	1.69	0.75
2:D:1962:DC:H1'	2:D:1963:DG:H5"	1.68	0.74
3:B:1624:THR:HG22	3:B:1660:LEU:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1435:ILE:HG22	3:B:1438:LEU:H	1.53	0.74
3:B:1456:TYR:O	3:B:1460:VAL:HG23	1.87	0.74
3:A:440:VAL:HG22	3:A:450:LEU:HD23	1.69	0.74
3:A:9:GLY:HA3	3:A:66:PHE:HB2	1.70	0.73
3:B:1678:THR:O	3:B:1682:GLU:HG3	1.89	0.73
3:B:1685:HIS:HE1	3:B:1707:ARG:H	1.35	0.73
3:B:1593:LEU:HD22	3:B:1692:LEU:HB3	1.69	0.73
3:B:1439:LYS:HB2	3:B:1451:GLU:HB3	1.71	0.73
3:B:1363:ARG:HH11	3:B:1363:ARG:HG2	1.52	0.72
3:A:92:LEU:HD12	3:A:116:LEU:HD12	1.70	0.72
3:B:1108:VAL:HG12	3:B:1109:ARG:N	2.01	0.72
3:B:1143:TRP:HH2	8:B:33:HOH:O	1.71	0.72
2:D:1968:DC:H2"	2:D:1969:DG:O5'	1.89	0.72
3:B:1027:TYR:CE1	3:B:1112:VAL:HG21	2.25	0.71
3:A:172:ARG:O	3:A:293:ARG:HD3	1.90	0.71
3:B:1426:GLU:O	3:B:1430:ARG:HG2	1.89	0.71
3:A:161:LYS:HD2	3:A:162:SER:N	2.06	0.71
3:A:331:ASP:OD2	3:A:334:ARG:HD2	1.89	0.71
3:A:579:VAL:HB	3:A:692:LEU:HD23	1.73	0.71
3:A:585:ASN:O	3:A:586:MET:HB2	1.91	0.71
3:B:1010:PRO:HG2	3:B:1011:GLY:H	1.56	0.71
3:B:1698:PHE:O	3:B:1701:THR:HB	1.91	0.70
3:A:312:PHE:HB3	3:A:319:ARG:HG3	1.72	0.70
1:C:1905:DC:H2"	1:C:1906:DG:H5'	1.73	0.70
3:A:581:ILE:HD11	3:A:692:LEU:HD22	1.74	0.70
3:A:678:THR:O	3:A:682:GLU:HG3	1.92	0.69
3:A:758:LEU:O	3:A:762:MET:HG3	1.92	0.69
3:A:171:PHE:CD2	3:A:254:GLU:HG3	2.27	0.69
3:B:1395:SER:O	3:B:1396:GLU:HB2	1.92	0.69
2:D:1967:DG:C2'	2:D:1968:DC:H5"	2.20	0.69
3:A:586:MET:HG2	3:B:1635:GLY:O	1.93	0.69
3:B:1011:GLY:HA3	3:B:1065:ASP:HB3	1.75	0.69
3:B:1282:ALA:HB3	3:B:1283:PRO:HD3	1.75	0.69
2:D:1965:DT:H2"	2:D:1966:DA:C8	2.28	0.69
3:B:1280:ARG:HG3	3:B:1280:ARG:HH11	1.58	0.69
3:B:1117:THR:CG2	3:B:1177:GLU:OE1	2.40	0.68
3:B:1426:GLU:HG3	3:B:1440:VAL:HG23	1.74	0.68
3:B:1153:GLY:O	3:B:1239:GLN:HG2	1.94	0.68
3:B:1016:LEU:HD11	3:B:1034:PHE:HE2	1.58	0.68
3:B:1318:LEU:O	3:B:1322:VAL:HG23	1.93	0.68
3:A:563:ARG:HA	3:A:563:ARG:NE	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:411:LEU:HB3	3:A:495:ILE:HG12	1.75	0.68
3:A:59:THR:HG22	3:A:60:HIS:N	2.07	0.68
3:A:584:PRO:HA	4:A:852:SO4:O4	1.94	0.68
3:A:438:LEU:HD21	3:A:450:LEU:HD22	1.74	0.68
3:B:1267:ARG:NE	3:B:1267:ARG:HA	2.09	0.68
3:A:161:LYS:HD2	3:A:162:SER:H	1.59	0.68
3:A:128:PRO:HB2	3:A:130:GLU:HG2	1.75	0.67
3:B:1122:LEU:H	3:B:1123:GLN:NE2	1.92	0.67
3:B:1597:ALA:HB2	3:B:1660:LEU:CD1	2.21	0.67
3:A:547:PHE:HA	3:A:616:LEU:O	1.95	0.67
3:A:60:HIS:CD2	3:A:60:HIS:N	2.63	0.67
3:A:661:LEU:HD13	3:A:664:VAL:HG21	1.77	0.67
3:B:1353:ARG:O	3:B:1357:GLN:HG3	1.94	0.67
3:A:267:ARG:HB2	3:A:269:GLN:NE2	2.08	0.66
2:D:1958:DC:C4'	3:B:1443:ASN:HD21	2.07	0.66
3:A:426:GLU:OE2	3:A:439:LYS:HA	1.95	0.66
3:B:1013:LEU:HD21	3:B:1021:VAL:HG21	1.78	0.66
3:B:1454:ARG:HH11	3:B:1457:TYR:HE2	1.44	0.66
3:A:174:ARG:HH21	3:A:264:GLU:CG	2.09	0.66
3:A:325:LEU:HD22	3:A:358:ILE:HG23	1.78	0.66
1:C:1916:DG:H2"	1:C:1917:DG:C5'	2.21	0.66
3:A:448:TYR:HD1	3:A:485:GLU:HG3	1.61	0.66
3:B:1001:MET:HB3	3:B:1004:MET:HB2	1.78	0.66
3:B:1454:ARG:HH11	3:B:1454:ARG:HG2	1.61	0.66
3:A:51:ALA:HA	3:A:56:LEU:HB2	1.77	0.66
3:A:556:GLY:O	3:A:569:PRO:HA	1.94	0.66
3:A:589:LYS:NZ	3:A:696:HIS:CE1	2.64	0.66
3:B:1158:THR:HG23	3:B:1160:LEU:HD11	1.78	0.66
3:B:1434:GLY:O	3:B:1436:PRO:HD3	1.95	0.65
2:D:1958:DC:H4'	3:B:1443:ASN:ND2	2.10	0.65
3:B:1460:VAL:HG11	3:B:1476:TYR:CZ	2.32	0.65
3:B:1525:ALA:O	3:B:1529:VAL:HG23	1.96	0.65
3:B:1169:GLU:O	3:B:1173:HIS:HD2	1.80	0.65
3:A:12:PRO:HD2	3:A:65:ASP:OD1	1.97	0.64
3:B:1160:LEU:N	3:B:1160:LEU:HD12	2.11	0.64
3:A:5:LEU:HD11	3:A:44:GLY:HA3	1.79	0.64
1:C:1921:DG:H2'	1:C:1922:DT:H71	1.79	0.64
3:B:1433:THR:HG22	3:B:1435:ILE:HG13	1.77	0.64
3:B:1454:ARG:HA	3:B:1457:TYR:CE2	2.32	0.64
3:B:1737:TYR:O	3:B:1741:VAL:HG23	1.98	0.64
3:A:479:PRO:HA	3:A:482:LYS:NZ	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:583:GLY:O	3:A:589:LYS:HE2	1.96	0.64
3:B:1399:LEU:HD21	3:B:1503:PHE:CD1	2.32	0.64
3:A:717:GLU:HG2	3:A:722:LEU:HD21	1.79	0.64
3:A:140:GLY:O	3:A:141:ASP:HB2	1.98	0.64
3:A:287:LEU:HD23	3:A:529:VAL:HG21	1.79	0.64
3:B:1287:LEU:O	3:B:1290:SER:HB3	1.98	0.64
3:B:1387:VAL:HG23	3:B:1399:LEU:O	1.97	0.64
3:B:1625:ARG:HH22	3:B:1627:GLY:HA2	1.63	0.64
3:A:636:LYS:HB3	3:B:1586:MET:HG2	1.79	0.63
3:A:722:LEU:N	3:A:744:MET:HE1	2.05	0.63
3:A:396:GLU:HG3	3:A:397:GLY:N	2.13	0.63
3:B:1005:LEU:HD21	3:B:1068:THR:HG21	1.79	0.63
3:B:1435:ILE:HG12	3:B:1456:TYR:CD2	2.33	0.63
3:B:1269:GLN:O	3:B:1270:ASP:HB2	1.99	0.63
3:B:1413:ALA:HA	3:B:1416:ARG:NH1	2.14	0.63
3:B:1711:LEU:HD23	3:B:1730:PRO:HA	1.81	0.63
3:B:1114:GLN:O	3:B:1115:LEU:HD23	1.99	0.62
3:A:353:ARG:O	3:A:357:GLN:HG3	1.99	0.62
3:A:405:ASP:HB3	3:A:408:LEU:HB3	1.80	0.62
3:A:74:PRO:HB2	3:A:76:ARG:HG2	1.81	0.62
1:C:1919:DT:OP1	3:A:475:ARG:NH1	2.29	0.62
2:D:1955:DG:H2'	2:D:1956:DA:H8	1.65	0.62
3:A:155:PHE:CZ	3:A:221:ARG:HG3	2.35	0.62
3:B:1297:LEU:O	3:B:1618:LEU:HD13	2.00	0.61
3:B:1363:ARG:NH1	3:B:1363:ARG:HG2	2.13	0.61
3:B:1122:LEU:H	3:B:1123:GLN:HE21	1.48	0.61
2:D:1960:DG:OP1	3:B:1470:LEU:HB3	2.00	0.61
3:A:550:ARG:HH11	3:A:550:ARG:HG3	1.64	0.61
3:A:708:LEU:HD23	3:A:708:LEU:C	2.21	0.61
3:B:1747:LEU:HD13	3:B:1748:PRO:HD2	1.82	0.61
3:B:1435:ILE:HG12	3:B:1456:TYR:HD2	1.64	0.61
3:B:1480:GLU:CD	3:B:1480:GLU:H	2.01	0.61
2:D:1962:DC:H2"	2:D:1963:DG:C5'	2.31	0.61
3:A:498:ARG:O	3:A:502:VAL:HG23	2.01	0.61
1:C:1901:DG:H1'	1:C:1902:DC:H5"	1.83	0.61
3:A:386:LEU:O	3:A:401:ARG:HG3	2.00	0.61
3:B:1674:VAL:HG22	3:B:1697:TYR:CD2	2.36	0.61
3:A:40:TYR:CE1	3:A:75:LEU:HD22	2.36	0.60
3:A:27:TYR:CE1	3:A:112:VAL:HG21	2.37	0.60
3:A:493:ALA:HA	3:A:496:ARG:NH1	2.15	0.60
3:B:1340:GLU:HA	3:B:1511:LYS:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:557:ARG:HH21	3:A:610:PRO:HA	1.62	0.60
3:B:1477:THR:CG2	3:B:1478:LEU:N	2.64	0.60
2:D:1955:DG:H2'	2:D:1956:DA:C8	2.37	0.60
3:A:548:GLY:O	3:A:617:PRO:HA	2.01	0.60
3:B:1450:LEU:O	3:B:1475:ARG:HA	2.01	0.60
1:C:1903:DG:H2"	1:C:1904:DA:H5"	1.83	0.60
3:A:440:VAL:HG22	3:A:450:LEU:CD2	2.30	0.60
2:D:1962:DC:H2"	2:D:1963:DG:H5'	1.84	0.60
2:D:1969:DG:H2"	2:D:1970:DT:C5'	2.31	0.60
3:A:225:LEU:HD21	3:A:238:LEU:HD11	1.82	0.60
3:A:239:GLN:NE2	3:A:240:PRO:HD2	2.16	0.60
3:B:1354:ARG:CZ	3:B:1358:ILE:HD12	2.31	0.60
3:B:1604:GLN:HE22	3:B:1619:PHE:H	1.50	0.60
3:A:114:GLN:HE22	3:A:123:GLN:HE22	1.49	0.60
3:B:1385:ALA:HB2	3:B:1404:TYR:CE1	2.36	0.60
3:A:376:SER:N	3:A:377:PRO:HD2	2.16	0.59
3:B:1716:ARG:HG3	3:B:1725:TYR:CE1	2.36	0.59
3:A:356:LEU:HA	3:A:359:LEU:HD13	1.83	0.59
3:A:375:LEU:C	3:A:377:PRO:HD2	2.23	0.59
3:A:674:VAL:HG11	3:A:699:GLU:HG3	1.84	0.59
3:B:1564:ARG:O	3:B:1565:THR:HG23	2.03	0.59
3:B:1161:LYS:N	3:B:1161:LYS:HD2	2.18	0.59
3:A:24:ARG:HA	3:A:32:LEU:HD22	1.83	0.59
3:A:636:LYS:HA	3:A:636:LYS:HE3	1.84	0.59
3:A:748:PRO:HB2	3:A:751:VAL:HG23	1.84	0.59
3:A:580:LEU:HD23	3:A:693:PHE:HB3	1.84	0.59
3:A:722:LEU:HB2	3:A:744:MET:CE	2.33	0.59
3:B:1353:ARG:HG3	3:B:1354:ARG:N	2.17	0.59
2:D:1960:DG:H2"	2:D:1961:DC:OP2	2.02	0.59
3:B:1287:LEU:HD23	3:B:1529:VAL:HG21	1.84	0.59
3:A:267:ARG:HB2	3:A:269:GLN:HE21	1.68	0.59
3:A:267:ARG:CB	3:A:269:GLN:HE21	2.15	0.59
3:A:156:LYS:NZ	3:A:173:HIS:HE1	2.01	0.59
3:B:1269:GLN:CD	3:B:1270:ASP:H	2.06	0.59
3:B:1097:GLN:HB3	3:B:1108:VAL:HG11	1.84	0.58
3:A:467:VAL:HG21	3:A:477:THR:OG1	2.04	0.58
3:A:674:VAL:HG13	3:A:699:GLU:HG3	1.85	0.58
3:A:160:LEU:HD12	3:A:160:LEU:N	2.18	0.58
3:A:557:ARG:HB2	3:A:610:PRO:HB2	1.84	0.58
3:A:35:GLN:HB3	3:A:96:ASP:HA	1.86	0.58
3:B:1585:ASN:O	3:B:1586:MET:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1967:DG:H2"	2:D:1968:DC:C5'	2.30	0.58
3:B:1376:SER:OG	3:B:1377:PRO:HD3	2.03	0.58
3:B:1628:ALA:O	3:B:1629:SER:O	2.22	0.58
3:B:1029:ASP:HB3	3:B:1091:ARG:NH2	2.18	0.58
3:B:1450:LEU:HD13	3:B:1464:TYR:CE2	2.39	0.58
3:A:170:LEU:HD12	3:A:198:PHE:CE2	2.39	0.57
3:A:363:ARG:HH22	3:A:374:ASP:HA	1.69	0.57
3:B:1547:PHE:HA	3:B:1616:LEU:O	2.04	0.57
1:C:1917:DG:H2"	1:C:1918:DC:OP2	2.03	0.57
3:A:551:LEU:HA	3:A:615:HIS:O	2.04	0.57
3:B:1269:GLN:CG	3:B:1270:ASP:H	2.17	0.57
3:A:336:ALA:O	3:A:340:GLU:HG3	2.04	0.57
3:A:416:ARG:HH11	3:A:416:ARG:HG2	1.68	0.57
3:B:1385:ALA:HB2	3:B:1404:TYR:CZ	2.39	0.57
3:B:1011:GLY:HA3	3:B:1065:ASP:CB	2.35	0.57
1:C:1901:DG:H2"	1:C:1902:DC:H5"	1.86	0.57
3:B:1430:ARG:HB3	3:B:1435:ILE:O	2.05	0.57
1:C:1921:DG:C2'	1:C:1922:DT:H71	2.35	0.57
3:A:363:ARG:HH22	3:A:374:ASP:CA	2.18	0.56
3:B:1066:PHE:HE2	3:B:1068:THR:HB	1.69	0.56
3:A:123:GLN:HB2	3:A:126:LEU:HD12	1.87	0.56
3:B:1469:THR:C	3:B:1470:LEU:HD12	2.25	0.56
3:B:1265:PRO:C	3:B:1267:ARG:H	2.09	0.56
3:B:1357:GLN:O	3:B:1360:PRO:HD2	2.05	0.56
3:A:394:VAL:HG13	3:A:395:SER:N	2.20	0.56
3:B:1485:GLU:C	3:B:1487:GLU:H	2.07	0.56
3:B:1625:ARG:O	3:B:1625:ARG:HG3	2.05	0.56
3:B:1356:LEU:O	3:B:1360:PRO:HD3	2.06	0.56
3:B:1747:LEU:CD1	3:B:1748:PRO:HD2	2.35	0.56
3:B:1232:GLN:O	3:B:1234:GLY:N	2.39	0.56
3:A:366:LEU:HD11	3:A:527:LEU:HD11	1.87	0.56
3:A:438:LEU:HD23	3:A:438:LEU:C	2.26	0.56
3:A:211:GLY:O	3:A:218:ARG:HD2	2.06	0.56
3:A:301:PRO:O	3:A:304:ALA:HB3	2.06	0.56
3:A:9:GLY:HA3	3:A:66:PHE:CB	2.35	0.56
3:B:1708:LEU:HD12	3:B:1709:LYS:H	1.70	0.56
3:A:366:LEU:CD1	3:A:527:LEU:HD11	2.36	0.55
3:A:463:GLU:CD	3:A:463:GLU:H	2.09	0.55
3:A:593:LEU:CD2	3:A:692:LEU:HB3	2.36	0.55
3:B:1661:LEU:HD22	3:B:1664:VAL:HG21	1.88	0.55
3:A:328:ARG:HB2	3:A:358:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:461:PRO:HG2	3:A:464:TYR:CD1	2.40	0.55
3:A:550:ARG:NH1	3:A:550:ARG:HG3	2.21	0.55
3:A:765:ARG:HH11	3:A:765:ARG:HG2	1.71	0.55
3:B:1580:LEU:HD12	3:B:1701:THR:HA	1.89	0.55
3:B:1758:LEU:O	3:B:1762:MET:HG3	2.06	0.55
3:B:1439:LYS:HD2	3:B:1451:GLU:OE1	2.06	0.55
3:B:1748:PRO:HB2	3:B:1751:VAL:HG23	1.89	0.55
3:B:1123:GLN:H	3:B:1123:GLN:NE2	2.05	0.55
3:A:412:ARG:O	3:A:416:ARG:HG3	2.07	0.55
3:A:491:LEU:O	3:A:495:ILE:HG13	2.07	0.55
3:B:1010:PRO:O	3:B:1011:GLY:O	2.25	0.55
3:B:1076:ARG:HG3	3:B:1077:ALA:H	1.71	0.55
3:B:1454:ARG:NH1	3:B:1457:TYR:HE2	2.05	0.55
3:B:1498:ARG:HD2	3:B:1501:GLU:OE1	2.07	0.55
3:A:593:LEU:HD22	3:A:692:LEU:HB3	1.88	0.55
3:B:1066:PHE:CE2	3:B:1068:THR:HB	2.42	0.55
3:A:276:LEU:O	3:A:536:VAL:HG21	2.06	0.54
3:B:1210:GLU:HG3	3:B:1225:LEU:HD12	1.88	0.54
3:B:1183:GLU:OE2	3:B:1219:ARG:NH2	2.33	0.54
3:B:1488:VAL:O	3:B:1492:GLU:HG3	2.06	0.54
3:A:267:ARG:CB	3:A:269:GLN:NE2	2.70	0.54
3:A:430:ARG:HD3	3:A:436:PRO:O	2.08	0.54
3:A:375:LEU:HD21	3:A:516:ALA:HB1	1.89	0.54
3:B:1097:GLN:NE2	3:B:1110:ARG:HH21	2.04	0.54
2:D:1951:DG:O5'	2:D:1951:DG:N2	2.40	0.54
3:A:225:LEU:CD2	3:A:238:LEU:HD11	2.37	0.54
3:B:1558:HIS:CD2	3:B:1561:VAL:H	2.25	0.54
3:A:379:LYS:HZ3	3:A:379:LYS:HB3	1.72	0.54
3:A:76:ARG:NH1	3:A:76:ARG:HB3	2.23	0.54
3:B:1685:HIS:CE1	3:B:1707:ARG:HB2	2.43	0.54
1:C:1901:DG:C2'	1:C:1902:DC:H5"	2.38	0.54
3:A:92:LEU:HB2	3:A:116:LEU:HB2	1.88	0.54
3:A:756:ARG:O	3:A:760:GLN:HG3	2.08	0.54
3:B:1143:TRP:HZ3	3:B:1161:LYS:O	1.91	0.54
3:A:454:ARG:HB3	3:A:455:PRO:HD3	1.89	0.54
3:A:685:HIS:HE1	3:A:707:ARG:H	1.54	0.54
3:A:392:LEU:HG	3:A:393:LYS:HG3	1.88	0.53
3:A:52:ARG:HG3	3:A:53:ALA:N	2.23	0.53
3:A:115:LEU:HB2	3:A:231:THR:HA	1.91	0.53
3:B:1076:ARG:HG3	3:B:1077:ALA:N	2.23	0.53
1:C:1923:DC:C2	2:D:1951:DG:N1	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:415:HIS:O	3:A:419:VAL:HG23	2.08	0.53
3:A:583:GLY:O	3:A:589:LYS:CE	2.57	0.53
3:B:1491:LEU:O	3:B:1495:ILE:HG13	2.09	0.53
3:A:100:PRO:HG2	3:A:103:GLU:CG	2.38	0.53
3:B:1097:GLN:HE21	3:B:1110:ARG:HH21	1.55	0.53
3:B:1110:ARG:HH11	3:B:1110:ARG:HG3	1.71	0.53
2:D:1961:DC:H2'	2:D:1962:DC:C5	2.44	0.53
3:B:1167:TYR:CD2	3:B:1198:PHE:HE1	2.27	0.53
3:B:1152:THR:HG23	3:B:1333:GLU:OE2	2.09	0.53
3:B:1339:LEU:HD23	3:B:1344:ALA:CB	2.39	0.53
3:A:234:GLY:HA3	8:A:1011:HOH:O	2.09	0.52
3:A:256:THR:HG23	3:A:260:LEU:HD22	1.91	0.52
3:B:1336:ALA:O	3:B:1340:GLU:HG3	2.09	0.52
3:B:1434:GLY:O	3:B:1436:PRO:CD	2.57	0.52
1:C:1919:DT:H3'	3:A:470:LEU:HD23	1.91	0.52
3:B:1042:CYS:O	3:B:1047:ALA:HB2	2.09	0.52
3:A:14:PRO:O	3:A:18:GLN:HB2	2.09	0.52
3:B:1040:TYR:CE1	3:B:1075:LEU:HD22	2.44	0.52
2:D:1951:DG:C2	2:D:1951:DG:OP2	2.63	0.52
2:D:1969:DG:H2"	2:D:1970:DT:H5"	1.91	0.52
3:A:35:GLN:HG2	3:A:97:GLN:H	1.74	0.52
3:A:704:GLY:O	3:A:705:LEU:HD23	2.09	0.52
3:A:539:ARG:HG2	3:A:540:TYR:CE2	2.44	0.52
3:A:556:GLY:HA3	3:A:595:GLN:NE2	2.25	0.52
3:A:712:HIS:CE1	3:A:729:LEU:HB2	2.45	0.52
3:A:574:MET:HG2	3:A:579:VAL:HG21	1.92	0.52
3:B:1092:LEU:HB2	3:B:1116:LEU:HB2	1.90	0.52
3:B:1477:THR:HG22	3:B:1478:LEU:N	2.25	0.52
3:A:239:GLN:HE21	3:A:240:PRO:HD2	1.73	0.52
3:A:357:GLN:HG2	3:A:379:LYS:HD2	1.91	0.52
3:B:1564:ARG:O	3:B:1565:THR:CG2	2.58	0.52
3:B:1685:HIS:CE1	3:B:1707:ARG:H	2.21	0.52
3:A:589:LYS:HZ2	3:A:696:HIS:CE1	2.26	0.51
3:B:1452:VAL:O	3:B:1473:ARG:HB2	2.09	0.51
3:A:16:LEU:HD11	3:A:110:ARG:NH1	2.25	0.51
3:A:271:THR:O	3:A:275:VAL:HG23	2.11	0.51
3:B:1137:ILE:HA	3:B:1144:GLY:O	2.10	0.51
1:C:1907:DC:H2"	1:C:1908:DT:O5'	2.10	0.51
3:A:469:THR:C	3:A:470:LEU:HD12	2.30	0.51
3:B:1122:LEU:HD21	3:B:1341:LEU:HD13	1.92	0.51
3:B:1602:LEU:O	3:B:1605:VAL:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1585:ASN:ND2	3:B:1589:LYS:NZ	2.58	0.51
3:B:1617:PRO:HG2	3:B:1619:PHE:CZ	2.44	0.51
3:A:734:SER:HB2	3:A:735:LYS:HD3	1.93	0.51
2:D:1959:DC:H1'	2:D:1960:DG:H5'	1.92	0.51
3:B:1110:ARG:NH1	3:B:1110:ARG:HG3	2.25	0.51
3:A:482:LYS:HD2	3:A:486:ARG:HH22	1.76	0.51
3:A:722:LEU:HB2	3:A:744:MET:HE3	1.93	0.51
3:B:1215:LEU:O	3:B:1219:ARG:HG3	2.11	0.51
3:A:490:ARG:HG2	3:A:490:ARG:NH1	2.22	0.51
3:B:1024:ARG:C	3:B:1024:ARG:HD2	2.30	0.51
3:A:379:LYS:NZ	3:A:379:LYS:HB3	2.26	0.51
3:B:1558:HIS:CD2	3:B:1561:VAL:HG23	2.46	0.51
3:A:299:ARG:NH1	3:A:303:GLU:OE1	2.44	0.51
3:A:502:VAL:O	3:A:506:VAL:HG23	2.11	0.51
3:B:1454:ARG:HD3	3:B:1457:TYR:CE2	2.46	0.51
2:D:1962:DC:C1'	2:D:1963:DG:H5"	2.39	0.51
3:A:118:PRO:HD2	3:A:201:MET:HE1	1.94	0.50
3:A:535:GLU:HG3	3:A:539:ARG:HH12	1.75	0.50
3:A:756:ARG:HG2	3:A:756:ARG:HH11	1.76	0.50
3:B:1123:GLN:HG3	3:B:1126:LEU:HD12	1.93	0.50
3:B:1434:GLY:HA3	8:B:37:HOH:O	2.11	0.50
3:A:249:PHE:CG	3:A:294:HIS:HB3	2.47	0.50
3:A:525:ALA:O	3:A:529:VAL:HG23	2.10	0.50
3:B:1415:HIS:CE1	3:B:1492:GLU:HG2	2.46	0.50
3:B:1473:ARG:HD3	3:B:1473:ARG:N	2.27	0.50
3:B:1760:GLN:O	3:B:1763:ALA:N	2.42	0.50
3:A:155:PHE:HZ	3:A:221:ARG:HG3	1.77	0.50
3:A:506:VAL:O	3:A:509:ARG:HB2	2.12	0.50
3:A:676:ILE:O	3:A:680:VAL:HG23	2.11	0.50
3:B:1435:ILE:C	3:B:1437:THR:H	2.14	0.50
3:B:1470:LEU:HD12	3:B:1470:LEU:N	2.27	0.50
3:B:1579:VAL:HB	3:B:1692:LEU:HD23	1.93	0.50
2:D:1955:DG:OP1	3:B:1015:PRO:HG2	2.12	0.50
3:B:1450:LEU:HD13	3:B:1464:TYR:CZ	2.47	0.50
3:B:1742:ALA:O	3:B:1745:ALA:HB3	2.12	0.50
2:D:1951:DG:C2	2:D:1951:DG:O5'	2.65	0.50
3:B:1129:ARG:HD2	3:B:1285:ARG:NH1	2.26	0.50
3:B:1502:VAL:O	3:B:1506:VAL:HG23	2.12	0.50
3:A:639:PHE:O	3:A:643:MET:HG2	2.12	0.49
3:B:1363:ARG:NH2	3:B:1368:GLU:HB2	2.26	0.49
3:B:1542:TYR:HA	3:B:1609:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:345:SER:HB2	3:A:346:PRO:HD2	1.94	0.49
3:B:1225:LEU:O	3:B:1229:GLN:HG3	2.12	0.49
3:B:1389:ASP:OD1	3:B:1389:ASP:O	2.29	0.49
3:A:405:ASP:OD1	3:A:498:ARG:NE	2.40	0.49
3:A:609:VAL:HB	3:A:610:PRO:HD2	1.92	0.49
3:A:555:ALA:HB3	3:A:612:GLU:HB2	1.94	0.49
3:A:482:LYS:HG2	3:A:486:ARG:HH12	1.78	0.49
3:B:1269:GLN:HE21	3:B:1270:ASP:H	1.58	0.49
3:B:1362:LEU:O	3:B:1366:LEU:HG	2.12	0.49
3:B:1537:ALA:HA	3:B:1542:TYR:HB2	1.94	0.49
3:B:1143:TRP:HB3	3:B:1166:LEU:HD13	1.95	0.49
3:B:1412:ARG:O	3:B:1416:ARG:HG3	2.12	0.49
3:B:1584:PRO:HB3	3:B:1737:TYR:CD1	2.47	0.49
3:A:320:GLU:O	3:A:324:ARG:HB2	2.13	0.49
3:A:590:SER:C	3:A:592:PHE:H	2.15	0.49
3:B:1030:TYR:N	3:B:1030:TYR:CD1	2.79	0.49
3:B:1181:ALA:HB1	3:B:1183:GLU:OE1	2.12	0.49
3:B:1346:PRO:HD2	3:B:1392:LEU:HB2	1.93	0.49
3:B:1451:GLU:HG3	3:B:1475:ARG:HG2	1.94	0.49
3:A:114:GLN:HE22	3:A:123:GLN:NE2	2.10	0.49
3:A:43:PHE:HA	3:A:47:ALA:HB2	1.95	0.49
3:B:1585:ASN:ND2	3:B:1589:LYS:HZ3	2.11	0.49
3:B:1711:LEU:CD2	3:B:1730:PRO:HA	2.43	0.49
3:B:1485:GLU:C	3:B:1487:GLU:N	2.65	0.49
3:B:1426:GLU:HG2	3:B:1430:ARG:CZ	2.43	0.48
1:C:1918:DC:H2"	1:C:1919:DT:H5'	1.94	0.48
2:D:1955:DG:H4'	2:D:1955:DG:OP1	2.13	0.48
3:B:1446:PHE:HB2	8:B:23:HOH:O	2.13	0.48
3:A:267:ARG:CG	3:A:269:GLN:NE2	2.77	0.48
3:A:282:ALA:HB3	3:A:283:PRO:HD3	1.94	0.48
3:A:640:MET:O	3:A:644:GLU:HG3	2.13	0.48
3:B:1001:MET:CE	3:B:1004:MET:HG3	2.43	0.48
3:B:1013:LEU:CD2	3:B:1021:VAL:HG21	2.42	0.48
3:B:1387:VAL:C	3:B:1389:ASP:H	2.17	0.48
3:B:1668:THR:OG1	3:B:1669:SER:N	2.46	0.48
1:C:1910:DG:OP1	3:B:1439:LYS:NZ	2.37	0.48
3:A:663:GLU:O	3:A:666:ARG:HG2	2.13	0.48
3:B:1299:ARG:NH2	3:B:1547:PHE:O	2.46	0.48
3:B:1574:MET:HG2	3:B:1579:VAL:HG21	1.95	0.48
3:A:318:LEU:HD11	3:A:366:LEU:CD2	2.39	0.48
3:A:24:ARG:CA	3:A:32:LEU:HD22	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1051:ALA:HA	3:B:1056:LEU:HB2	1.96	0.48
1:C:1902:DC:H2"	1:C:1903:DG:C8	2.47	0.48
3:A:16:LEU:CD1	3:A:110:ARG:NH1	2.76	0.48
3:A:356:LEU:HD21	3:A:375:LEU:HD13	1.96	0.48
3:A:493:ALA:HA	3:A:496:ARG:HH12	1.78	0.48
3:A:66:PHE:CD2	3:A:66:PHE:C	2.86	0.48
3:B:1417:GLU:O	3:B:1420:ALA:HB3	2.13	0.48
3:B:1429:GLU:C	3:B:1431:GLU:N	2.67	0.48
3:B:1429:GLU:O	3:B:1431:GLU:N	2.47	0.48
3:B:1554:ARG:HH11	3:B:1554:ARG:HG2	1.78	0.48
3:B:1678:THR:HA	3:B:1700:LEU:HD21	1.96	0.48
3:A:14:PRO:HD2	3:A:17:LEU:HD12	1.96	0.48
3:A:95:ALA:HA	3:A:112:VAL:HA	1.95	0.48
3:B:1370:VAL:CG1	3:B:1523:ILE:HG21	2.44	0.48
3:A:590:SER:C	3:A:592:PHE:N	2.68	0.48
3:B:1098:VAL:HG21	3:B:1109:ARG:HG2	1.95	0.48
3:B:1143:TRP:CZ2	3:B:1163:LYS:HB2	2.48	0.48
3:B:1388:GLU:HG3	3:B:1401:ARG:HH22	1.79	0.48
3:B:1429:GLU:C	3:B:1431:GLU:H	2.17	0.48
3:A:479:PRO:HA	3:A:482:LYS:HZ3	1.77	0.48
3:B:1033:LEU:HD23	3:B:1042:CYS:SG	2.54	0.48
3:A:59:THR:CG2	3:A:60:HIS:H	2.11	0.47
3:B:1152:THR:HG22	3:B:1154:GLU:H	1.79	0.47
3:B:1174:ARG:HD3	3:B:1174:ARG:HA	1.66	0.47
3:B:1363:ARG:HH12	3:B:1367:GLY:HA2	1.79	0.47
1:C:1920:DC:H4'	3:B:1445:VAL:HG13	1.95	0.47
2:D:1969:DG:H2"	2:D:1970:DT:O5'	2.14	0.47
3:A:267:ARG:O	3:A:269:GLN:N	2.47	0.47
3:A:454:ARG:HA	3:A:457:TYR:CE1	2.48	0.47
3:A:554:ARG:O	3:A:612:GLU:HB2	2.13	0.47
3:B:1115:LEU:HB2	3:B:1231:THR:HA	1.95	0.47
3:B:1594:ARG:HH11	3:B:1626:ILE:HG21	1.78	0.47
3:A:718:GLU:O	3:A:719:ALA:C	2.52	0.47
3:B:1345:SER:HB2	3:B:1392:LEU:HD13	1.95	0.47
3:B:1450:LEU:O	3:B:1476:TYR:N	2.47	0.47
3:B:1563:ARG:HA	3:B:1563:ARG:NH1	2.28	0.47
3:A:394:VAL:HG21	3:A:500:GLU:CA	2.42	0.47
3:B:1200:VAL:O	3:B:1202:LEU:HD13	2.14	0.47
3:B:1345:SER:O	3:B:1348:ASP:HB2	2.14	0.47
3:A:390:PRO:HA	3:A:391:PRO:HD3	1.76	0.47
3:A:539:ARG:HG2	3:A:540:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:751:VAL:HG21	3:B:1650:LEU:HD13	1.96	0.47
3:A:83:GLU:CG	3:A:87:LYS:HE2	2.44	0.47
3:B:1580:LEU:HD23	3:B:1693:PHE:HB3	1.96	0.47
2:D:1970:DT:H2"	2:D:1971:DC:C5	2.50	0.47
3:A:354:ARG:HH11	3:A:354:ARG:HG2	1.79	0.47
1:C:1904:DA:H2	2:D:1971:DC:O2	1.96	0.47
3:B:1256:THR:HA	3:B:1624:THR:OG1	2.14	0.47
3:B:1735:LYS:HB3	3:B:1735:LYS:HE2	1.70	0.47
3:A:114:GLN:NE2	3:A:123:GLN:HE22	2.13	0.47
3:B:1026:GLN:O	3:B:1028:PRO:HD2	2.14	0.47
1:C:1909:DA:OP1	3:B:1455:PRO:HD3	2.15	0.47
3:A:100:PRO:HG2	3:A:103:GLU:HG3	1.97	0.47
3:A:734:SER:CB	3:A:735:LYS:HD3	2.44	0.47
3:B:1027:TYR:HE1	3:B:1112:VAL:HG21	1.75	0.47
3:B:1116:LEU:N	3:B:1116:LEU:HD12	2.30	0.47
3:B:1359:LEU:HB3	3:B:1360:PRO:HD3	1.96	0.47
3:B:1388:GLU:O	3:B:1389:ASP:HB2	2.15	0.47
3:B:1454:ARG:HG2	3:B:1454:ARG:NH1	2.27	0.47
3:B:1564:ARG:HE	3:B:1564:ARG:HB2	1.52	0.47
3:B:1636:LYS:HG2	3:B:1640:MET:CE	2.45	0.47
3:B:1623:TYR:HE2	3:B:1652:GLU:OE2	1.97	0.47
3:B:1685:HIS:HE1	3:B:1707:ARG:N	2.09	0.47
3:A:415:HIS:CE1	3:A:488:VAL:HG13	2.49	0.46
3:A:5:LEU:HG	3:A:6:LYS:N	2.30	0.46
3:A:408:LEU:HD21	3:A:412:ARG:HH12	1.80	0.46
3:A:474:GLN:HG2	3:A:476:TYR:OH	2.15	0.46
3:A:11:GLY:HA3	3:A:65:ASP:HB3	1.96	0.46
3:B:1163:LYS:HG3	3:B:1167:TYR:CE1	2.50	0.46
3:B:1011:GLY:CA	3:B:1065:ASP:HB3	2.45	0.46
3:B:1315:GLU:HB3	3:B:1318:LEU:HB3	1.97	0.46
3:B:1687:ARG:O	3:B:1688:ARG:HB2	2.16	0.46
2:D:1951:DG:P	2:D:1951:DG:N2	2.89	0.46
3:B:1357:GLN:HA	3:B:1379:LYS:HD2	1.98	0.46
3:B:1346:PRO:HB3	3:B:1399:LEU:HD11	1.98	0.46
3:B:1551:LEU:HD23	3:B:1551:LEU:C	2.35	0.46
3:B:1678:THR:HG23	3:B:1703:LEU:HD11	1.96	0.46
2:D:1955:DG:C2'	2:D:1956:DA:C8	2.99	0.46
3:A:564:ARG:O	3:A:565:THR:OG1	2.30	0.46
3:B:1370:VAL:HG13	3:B:1523:ILE:HG21	1.97	0.46
3:B:1654:THR:O	3:B:1689:ALA:HB2	2.15	0.46
3:B:1269:GLN:CG	3:B:1270:ASP:N	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1356:LEU:HB3	3:B:1379:LYS:HB2	1.98	0.46
3:B:1272:LEU:HD22	3:B:1598:LEU:HD22	1.97	0.46
1:C:1912:DG:O6	2:D:1962:DC:N4	2.46	0.46
3:A:172:ARG:HD2	3:A:294:HIS:NE2	2.31	0.46
3:B:1129:ARG:HD2	3:B:1285:ARG:CZ	2.46	0.46
3:B:1145:LEU:HD21	3:B:1170:LEU:HD23	1.97	0.46
3:A:450:LEU:HA	3:A:450:LEU:HD23	1.84	0.46
3:A:623:TYR:CE2	3:A:652:GLU:OE2	2.69	0.46
3:B:1068:THR:OG1	3:B:1069:PRO:HD2	2.15	0.46
3:B:1346:PRO:HB3	3:B:1399:LEU:CD1	2.46	0.46
2:D:1958:DC:C3'	3:B:1443:ASN:HD21	2.28	0.46
3:B:1470:LEU:HB2	3:B:1473:ARG:O	2.16	0.46
2:D:1962:DC:C2'	2:D:1963:DG:H5"	2.46	0.46
3:A:256:THR:CG2	3:A:260:LEU:HD22	2.45	0.46
3:A:35:GLN:HG2	3:A:97:GLN:N	2.30	0.46
3:A:356:LEU:HD11	3:A:378:LEU:HD13	1.98	0.46
3:A:581:ILE:HD13	3:A:592:PHE:HD2	1.80	0.46
3:A:322:VAL:O	3:A:326:LEU:HG	2.15	0.46
3:A:335:LEU:HD21	3:A:348:ASP:HB3	1.98	0.46
3:A:570:ASN:ND2	3:A:728:VAL:HG23	2.31	0.46
3:A:591:THR:O	3:A:591:THR:HG22	2.15	0.46
3:B:1559:PRO:HD3	3:B:1610:PRO:HG3	1.98	0.46
3:A:654:THR:C	3:A:656:ASN:H	2.18	0.45
3:B:1167:TYR:CD2	3:B:1197:ARG:HD3	2.51	0.45
2:D:1958:DC:O3'	3:B:1443:ASN:ND2	2.48	0.45
3:A:627:GLY:O	3:A:628:ALA:C	2.54	0.45
3:B:1429:GLU:O	3:B:1432:ARG:N	2.49	0.45
3:B:1604:GLN:HE22	3:B:1619:PHE:N	2.13	0.45
3:B:1268:GLY:O	3:B:1269:GLN:O	2.34	0.45
3:B:1356:LEU:HD11	3:B:1378:LEU:HD13	1.99	0.45
3:B:1739:VAL:HG21	3:B:1759:LEU:HD11	1.98	0.45
3:B:1740:GLU:O	3:B:1743:ALA:HB3	2.17	0.45
3:A:565:THR:CG2	3:A:566:GLU:N	2.79	0.45
3:A:54:LEU:HD13	3:A:81:TYR:CD1	2.51	0.45
3:B:1098:VAL:O	3:B:1099:GLU:C	2.54	0.45
3:B:1453:THR:OG1	3:B:1455:PRO:HD2	2.16	0.45
3:B:1454:ARG:HD3	3:B:1457:TYR:CD2	2.51	0.45
3:B:1594:ARG:NH1	3:B:1626:ILE:HG21	2.31	0.45
1:C:1901:DG:C1'	1:C:1902:DC:H5"	2.47	0.45
1:C:1923:DC:C2	2:D:1951:DG:C6	3.05	0.45
3:A:309:VAL:O	3:A:313:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1099:GLU:O	3:B:1100:PRO:C	2.54	0.45
2:D:1971:DC:C2'	2:D:1972:DG:H5"	2.46	0.45
3:A:172:ARG:HH22	3:A:252:LEU:H	1.64	0.45
3:A:35:GLN:NE2	3:A:37:GLY:O	2.48	0.45
3:A:739:VAL:HG12	3:A:752:VAL:HG13	1.97	0.45
3:B:1388:GLU:HG3	3:B:1401:ARG:NH2	2.32	0.45
1:C:1904:DA:H2"	1:C:1905:DC:H5"	1.98	0.45
3:B:1217:LEU:HD23	3:B:1217:LEU:HA	1.68	0.45
3:B:1551:LEU:HG	3:B:1616:LEU:HD23	1.98	0.45
2:D:1958:DC:H2"	2:D:1959:DC:C5	2.52	0.45
3:A:385:ALA:O	3:A:400:ILE:HA	2.17	0.45
3:A:442:TYR:HE1	3:A:489:TYR:HH	1.64	0.45
3:B:1215:LEU:HD23	3:B:1218:ARG:NH1	2.32	0.45
3:A:42:CYS:O	3:A:47:ALA:HB2	2.17	0.45
3:B:1035:GLN:O	3:B:1110:ARG:NE	2.47	0.45
3:B:1119:GLY:O	3:B:1134:LEU:HB2	2.16	0.45
3:B:1143:TRP:CH2	8:B:33:HOH:O	2.56	0.45
3:B:1554:ARG:NH1	3:B:1613:GLU:OE1	2.50	0.45
3:B:1339:LEU:O	3:B:1511:LYS:HD2	2.17	0.44
3:A:278:GLU:HG3	3:A:536:VAL:CG2	2.47	0.44
3:B:1114:GLN:NE2	8:B:26:HOH:O	2.50	0.44
3:B:1267:ARG:HE	3:B:1267:ARG:HA	1.80	0.44
3:A:637:SER:OG	3:A:638:THR:N	2.50	0.44
3:B:1663:GLU:OE1	3:B:1696:HIS:ND1	2.50	0.44
1:C:1912:DG:H2"	1:C:1913:DT:OP2	2.17	0.44
3:A:121:LEU:HD13	3:A:126:LEU:HB3	1.98	0.44
3:A:490:ARG:CG	3:A:490:ARG:HH11	2.24	0.44
3:A:584:PRO:O	3:A:587:ALA:HB3	2.17	0.44
3:A:160:LEU:HD21	3:A:169:GLU:HG3	2.00	0.44
3:A:377:PRO:HG2	3:A:378:LEU:H	1.82	0.44
3:B:1149:ASP:OD1	3:B:1149:ASP:C	2.56	0.44
3:B:1438:LEU:HD13	3:B:1452:VAL:HG22	1.99	0.44
3:B:1685:HIS:HD2	3:B:1686:GLU:OE2	2.00	0.44
2:D:1959:DC:H2"	2:D:1960:DG:H5'	1.99	0.44
3:B:1167:TYR:H	3:B:1167:TYR:HD1	1.65	0.44
3:B:1390:PRO:HA	3:B:1391:PRO:HD3	1.89	0.44
3:B:1615:HIS:N	3:B:1615:HIS:CD2	2.85	0.44
3:B:1617:PRO:HG2	3:B:1619:PHE:CE2	2.52	0.44
3:A:717:GLU:HG2	3:A:722:LEU:CD2	2.46	0.44
3:A:35:GLN:CB	3:A:96:ASP:HA	2.46	0.44
3:B:1236:LEU:HB2	3:B:1238:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1671:LEU:HD12	8:B:69:HOH:O	2.18	0.44
3:A:54:LEU:HD13	3:A:81:TYR:HD1	1.81	0.43
3:B:1366:LEU:HB3	3:B:1370:VAL:HG21	2.00	0.43
3:B:1478:LEU:CD2	3:B:1480:GLU:OE2	2.66	0.43
3:A:668:THR:HG23	3:A:669:SER:N	2.33	0.43
3:B:1122:LEU:HD21	3:B:1341:LEU:CD1	2.48	0.43
3:A:191:LEU:HG	3:A:195:ARG:NH1	2.34	0.43
3:A:26:GLN:C	3:A:28:PRO:HD3	2.39	0.43
3:A:482:LYS:CG	3:A:486:ARG:HH22	2.31	0.43
3:B:1581:ILE:HG22	3:B:1589:LYS:HG2	2.01	0.43
3:B:1604:GLN:NE2	3:B:1619:PHE:H	2.14	0.43
3:A:139:THR:OG1	3:A:183:GLU:OE2	2.36	0.43
3:A:35:GLN:HB2	3:A:40:TYR:CE2	2.53	0.43
3:A:541:GLY:O	3:A:557:ARG:NH2	2.52	0.43
3:B:1464:TYR:HD2	3:B:1476:TYR:CB	2.31	0.43
3:B:1400:ILE:HG12	3:B:1499:GLU:HG3	2.01	0.43
3:A:273:PHE:HD1	3:A:292:LEU:HD12	1.83	0.43
3:B:1478:LEU:HD23	3:B:1480:GLU:OE2	2.19	0.43
3:B:1260:LEU:HD21	3:B:1597:ALA:HB1	1.99	0.43
1:C:1905:DC:H2"	1:C:1906:DG:C5'	2.45	0.43
3:B:1440:VAL:HG22	3:B:1450:LEU:HD23	1.99	0.43
3:B:1708:LEU:HD12	3:B:1709:LYS:N	2.34	0.43
3:A:396:GLU:O	3:A:397:GLY:O	2.36	0.43
3:B:1010:PRO:HG2	3:B:1011:GLY:N	2.29	0.43
3:B:1467:VAL:HG21	3:B:1477:THR:OG1	2.19	0.43
3:B:1497:ARG:O	3:B:1501:GLU:HG3	2.19	0.43
3:B:1625:ARG:HG2	3:B:1664:VAL:HG22	1.99	0.43
3:A:287:LEU:HD23	3:A:529:VAL:CG2	2.48	0.43
3:A:685:HIS:CE1	3:A:707:ARG:HB2	2.54	0.43
3:B:1314:ARG:HH11	3:B:1314:ARG:HG3	1.84	0.43
3:A:393:LYS:O	3:A:396:GLU:HG2	2.19	0.43
3:A:416:ARG:NH1	3:A:416:ARG:HG2	2.31	0.43
3:A:557:ARG:NH2	3:A:610:PRO:CA	2.68	0.43
3:B:1228:ALA:HB3	3:B:1236:LEU:HD11	2.01	0.43
3:B:1282:ALA:O	3:B:1283:PRO:C	2.58	0.43
3:A:34:PHE:O	3:A:40:TYR:HA	2.19	0.42
3:A:670:SER:O	3:A:674:VAL:HG23	2.19	0.42
3:A:717:GLU:HA	3:A:722:LEU:HD23	2.01	0.42
3:A:76:ARG:CB	3:A:76:ARG:HH11	2.32	0.42
3:B:1067:THR:O	3:B:1067:THR:HG23	2.19	0.42
3:B:1462:LYS:C	3:B:1464:TYR:N	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1470:LEU:CD2	3:B:1473:ARG:HE	2.32	0.42
3:A:145:LEU:HD22	3:A:146:ALA:N	2.35	0.42
3:A:174:ARG:NH2	3:A:264:GLU:HG2	2.27	0.42
3:A:129:ARG:HD3	3:A:285:ARG:NH1	2.34	0.42
3:A:99:GLU:HB2	3:A:109:ARG:NH2	2.34	0.42
3:B:1394:VAL:O	3:B:1395:SER:HB3	2.19	0.42
3:B:1623:TYR:HE2	3:B:1652:GLU:CD	2.22	0.42
3:A:191:LEU:HG	3:A:195:ARG:HH12	1.83	0.42
3:A:49:ARG:HG2	3:A:49:ARG:HH11	1.84	0.42
3:B:1280:ARG:HG3	3:B:1280:ARG:NH1	2.30	0.42
3:B:1551:LEU:HD12	3:B:1619:PHE:HZ	1.84	0.42
3:A:239:GLN:O	3:A:240:PRO:C	2.55	0.42
3:A:375:LEU:HD21	3:A:516:ALA:CB	2.49	0.42
3:A:729:LEU:HB3	3:A:730:PRO:HD2	2.01	0.42
3:B:1181:ALA:HA	3:B:1207:PHE:CE1	2.54	0.42
3:B:1192:ASP:O	3:B:1196:LYS:HG3	2.18	0.42
3:B:1353:ARG:NH2	3:B:1388:GLU:HA	2.35	0.42
1:C:1913:DT:H6	1:C:1913:DT:H2'	1.70	0.42
3:A:145:LEU:HD11	3:A:147:PHE:CZ	2.55	0.42
3:A:225:LEU:HD21	3:A:238:LEU:CD1	2.48	0.42
3:B:1036:VAL:HG12	3:B:1036:VAL:O	2.19	0.42
3:B:1120:THR:O	3:B:1150:VAL:HG21	2.20	0.42
3:B:1359:LEU:N	3:B:1360:PRO:CD	2.82	0.42
3:A:16:LEU:CD1	3:A:110:ARG:HH12	2.31	0.42
3:B:1508:GLU:O	3:B:1512:ARG:HG3	2.20	0.42
2:D:1955:DG:C2'	2:D:1956:DA:H8	2.30	0.42
3:A:372:LEU:HD21	3:A:524:LEU:CD2	2.50	0.42
3:A:551:LEU:O	3:A:573:GLU:HA	2.19	0.42
3:B:1232:GLN:CG	3:B:1232:GLN:O	2.67	0.42
3:B:1518:ARG:HH11	3:B:1518:ARG:HG2	1.85	0.42
3:B:1696:HIS:NE2	4:B:1852:SO4:O4	2.52	0.42
3:A:160:LEU:HD23	3:A:165:ALA:HB1	2.01	0.42
3:A:431:GLU:OE1	3:A:431:GLU:HA	2.20	0.42
3:A:722:LEU:HB2	3:A:744:MET:HE1	2.02	0.42
3:A:169:GLU:O	3:A:173:HIS:HD2	2.02	0.42
3:A:677:ALA:CB	3:A:700:LEU:HD11	2.39	0.42
3:A:83:GLU:O	3:A:87:LYS:HG3	2.20	0.42
3:B:1023:LEU:O	3:B:1024:ARG:C	2.57	0.42
3:B:1421:TYR:CD2	3:B:1421:TYR:C	2.92	0.42
3:A:237:SER:OG	3:A:340:GLU:OE1	2.34	0.42
3:A:16:LEU:HD11	3:A:34:PHE:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:449:TYR:C	3:A:449:TYR:CD1	2.92	0.42
3:A:6:LYS:NZ	3:A:45:GLU:HG2	2.34	0.42
3:B:1022:GLU:O	3:B:1026:GLN:HG3	2.19	0.42
3:B:1073:ILE:O	3:B:1073:ILE:HG13	2.20	0.42
3:B:1636:LYS:HG2	3:B:1640:MET:HE3	2.02	0.42
3:B:1670:SER:O	3:B:1674:VAL:HG23	2.20	0.42
1:C:1918:DC:H2"	1:C:1919:DT:C5'	2.49	0.42
3:A:465:ARG:O	3:A:476:TYR:HA	2.20	0.41
3:A:35:GLN:CG	3:A:97:GLN:HG3	2.39	0.41
3:B:1174:ARG:N	3:B:1175:PRO:HD3	2.35	0.41
3:B:1178:VAL:HG23	3:B:1200:VAL:HG11	2.02	0.41
3:B:1465:ARG:HG3	3:B:1465:ARG:HH11	1.85	0.41
3:B:1485:GLU:O	3:B:1487:GLU:N	2.53	0.41
3:B:1558:HIS:O	3:B:1562:GLU:HG2	2.20	0.41
3:B:1595:GLN:HG3	3:B:1596:THR:N	2.35	0.41
3:A:200:VAL:HG12	3:A:201:MET:N	2.35	0.41
3:A:58:LEU:HD23	3:A:58:LEU:HA	1.81	0.41
3:A:688:ARG:HG2	3:A:688:ARG:HH11	1.84	0.41
3:B:1024:ARG:HD2	3:B:1024:ARG:O	2.20	0.41
3:B:1470:LEU:HD22	3:B:1473:ARG:NE	2.35	0.41
3:B:1558:HIS:HB3	3:B:1561:VAL:HB	2.02	0.41
3:B:1692:LEU:HD23	3:B:1692:LEU:HA	1.62	0.41
3:B:1097:GLN:HE21	3:B:1110:ARG:NH2	2.17	0.41
3:B:1309:VAL:O	3:B:1313:VAL:HG23	2.20	0.41
3:A:585:ASN:HA	3:A:585:ASN:HD22	1.72	0.41
3:A:747:LEU:HD22	3:A:748:PRO:HD2	2.02	0.41
3:B:1188:GLY:O	3:B:1192:ASP:OD1	2.39	0.41
3:B:1433:THR:HG22	3:B:1433:THR:O	2.21	0.41
1:C:1910:DG:H2"	1:C:1911:DC:OP2	2.21	0.41
1:C:1920:DC:H2"	1:C:1921:DG:C8	2.55	0.41
3:A:335:LEU:HD22	3:A:335:LEU:HA	1.90	0.41
3:B:1213:GLY:O	3:B:1218:ARG:HD2	2.21	0.41
3:B:1232:GLN:HG2	3:B:1341:LEU:HD22	2.03	0.41
3:A:260:LEU:HA	3:A:260:LEU:HD12	1.93	0.41
3:A:34:PHE:O	3:A:41:GLU:N	2.43	0.41
3:A:464:TYR:HB3	3:A:476:TYR:CG	2.56	0.41
3:A:394:VAL:HG11	3:A:500:GLU:HG3	2.02	0.41
3:A:83:GLU:HG2	3:A:87:LYS:HE2	2.02	0.41
3:B:1693:PHE:CE2	3:B:1695:THR:HB	2.55	0.41
2:D:1962:DC:C2'	2:D:1963:DG:C5'	2.98	0.41
3:B:1366:LEU:HD13	3:B:1370:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:332:LEU:HD11	3:A:355:SER:HB3	2.03	0.41
3:B:1005:LEU:CD2	3:B:1068:THR:HG21	2.47	0.41
3:A:16:LEU:HD11	3:A:110:ARG:HH12	1.85	0.41
3:A:379:LYS:HE2	3:A:383:GLU:OE2	2.20	0.41
3:A:24:ARG:HD2	3:A:46:ASP:OD2	2.20	0.41
3:A:381:GLU:OE2	3:A:509:ARG:HD3	2.20	0.41
3:A:585:ASN:HD21	3:A:696:HIS:HE1	1.69	0.41
3:A:642:GLU:O	3:A:646:VAL:HG23	2.21	0.41
3:B:1123:GLN:CG	3:B:1126:LEU:HD12	2.51	0.41
3:B:1178:VAL:HG12	3:B:1179:LEU:N	2.36	0.41
3:B:1375:LEU:HD21	3:B:1516:ALA:HB1	2.02	0.41
3:B:1375:LEU:HD21	3:B:1516:ALA:CB	2.50	0.41
2:D:1952:DG:H2"	2:D:1953:DA:OP2	2.21	0.41
1:C:1908:DT:H3	2:D:1966:DA:H61	1.69	0.41
3:B:1013:LEU:HD12	3:B:1013:LEU:HA	1.83	0.41
3:B:1345:SER:HB2	3:B:1392:LEU:HD22	2.03	0.41
3:B:1558:HIS:HD2	3:B:1561:VAL:H	1.66	0.41
3:A:406:PRO:HG2	3:A:407:ASP:H	1.86	0.40
3:A:56:LEU:HD21	3:A:73:ILE:HG22	2.02	0.40
3:B:1247:GLY:HA2	3:B:1251:ARG:CZ	2.52	0.40
3:B:1747:LEU:HD13	3:B:1748:PRO:CD	2.50	0.40
3:B:1590:SER:OG	5:B:1998:BEF:F3	2.29	0.40
3:A:678:THR:HA	3:A:700:LEU:CD2	2.51	0.40
3:B:1663:GLU:OE1	3:B:1696:HIS:CE1	2.75	0.40
3:A:396:GLU:CG	3:A:397:GLY:N	2.81	0.40
3:A:750:GLU:CD	3:A:750:GLU:H	2.24	0.40
3:B:1002:GLU:OE1	3:B:1002:GLU:N	2.53	0.40
3:B:1170:LEU:HD22	3:B:1170:LEU:HA	1.83	0.40
3:B:1206:PRO:O	3:B:1223:ALA:HA	2.22	0.40
3:B:1292:LEU:HA	3:B:1292:LEU:HD23	1.83	0.40
3:B:1332:LEU:HG	3:B:1517:LEU:HD22	2.02	0.40
3:B:1437:THR:O	3:B:1438:LEU:C	2.59	0.40
3:A:412:ARG:HH11	3:A:412:ARG:HG3	1.86	0.40
3:A:435:ILE:HG23	3:A:456:TYR:CD2	2.56	0.40
3:B:1232:GLN:OE1	3:B:1343:ARG:NE	2.54	0.40
3:B:1585:ASN:HD22	3:B:1589:LYS:NZ	2.18	0.40
3:A:376:SER:N	3:A:377:PRO:CD	2.82	0.40
3:A:357:GLN:HA	3:A:379:LYS:HD2	2.03	0.40
3:B:1661:LEU:HD11	3:B:1684:LEU:CD1	2.52	0.40
3:B:1661:LEU:HD11	3:B:1684:LEU:HD12	2.03	0.40
3:B:1701:THR:O	3:B:1701:THR:CG2	2.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1972:DG:O3'	3:A:427:GLU:OE2[3_856]	2.18	0.02

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	
3	A	755/765 (99%)	681 (90%)	62 (8%)	12 (2%)	9	36
3	B	755/765 (99%)	660 (87%)	73 (10%)	22 (3%)	4	23
All	All	1510/1530 (99%)	1341 (89%)	135 (9%)	34 (2%)	6	28

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	719	ALA
3	B	1010	PRO
3	B	1011	GLY
3	B	1108	VAL
3	B	1110	ARG
3	B	1233	GLY
3	B	1269	GLN
3	B	1396	GLU
3	B	1629	SER
3	A	98	VAL
3	A	141	ASP
3	A	187	ASN
3	A	268	GLY
3	A	397	GLY
3	A	703	LEU
3	B	1109	ARG
3	B	1140	GLY

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Mol	Chain	Res	Type
3	B	1391	PRO
3	B	1628	ALA
3	A	3	GLY
3	B	1438	LEU
3	B	1575	ALA
3	A	10	PRO
3	A	50	LEU
3	B	1078	PHE
3	B	1389	ASP
3	B	1267	ARG
3	B	1315	GLU
3	B	1435	ILE
3	A	51	ALA
3	B	1209	PRO
3	B	1486	ARG
3	B	1394	VAL
3	A	209	PRO

5.3.2 Protein sidechains (i)

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
3	A	613/617 (99%)	575 (94%)	38 (6%)	18 48
3	B	608/617 (98%)	564 (93%)	44 (7%)	14 43
All	All	1221/1234 (99%)	1139 (93%)	82 (7%)	16 45

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1	MET
3	A	18	GLN
3	A	35	GLN
3	A	58	LEU
3	A	60	HIS
3	A	66	PHE

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Mol	Chain	Res	Type
3	A	99	GLU
3	A	112	VAL
3	A	130	GLU
3	A	145	LEU
3	A	161	LYS
3	A	195	ARG
3	A	196	LYS
3	A	215	LEU
3	A	243	PHE
3	A	260	LEU
3	A	274	SER
3	A	276	LEU
3	A	335	LEU
3	A	363	ARG
3	A	378	LEU
3	A	509	ARG
3	A	527	LEU
3	A	563	ARG
3	A	578	LEU
3	A	582	THR
3	A	605	VAL
3	A	625	ARG
3	A	636	LYS
3	A	660	LEU
3	A	666	ARG
3	A	672	ASP
3	A	674	VAL
3	A	693	PHE
3	A	699	GLU
3	A	716	ARG
3	A	735	LYS
3	A	747	LEU
3	B	1006	LYS
3	B	1013	LEU
3	B	1018	GLN
3	B	1030	TYR
3	B	1070	MET
3	B	1075	LEU
3	B	1115	LEU
3	B	1117	THR
3	B	1122	LEU
3	B	1123	GLN

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Mol	Chain	Res	Type
3	B	1145	LEU
3	B	1161	LYS
3	B	1170	LEU
3	B	1183	GLU
3	B	1192	ASP
3	B	1217	LEU
3	B	1238	LEU
3	B	1276	LEU
3	B	1289	GLN
3	B	1314	ARG
3	B	1315	GLU
3	B	1332	LEU
3	B	1358	ILE
3	B	1363	ARG
3	B	1378	LEU
3	B	1391	PRO
3	B	1396	GLU
3	B	1446	PHE
3	B	1454	ARG
3	B	1473	ARG
3	B	1480	GLU
3	B	1484	LYS
3	B	1505	GLU
3	B	1546	ARG
3	B	1557	ARG
3	B	1563	ARG
3	B	1564	ARG
3	B	1605	VAL
3	B	1648	LEU
3	B	1663	GLU
3	B	1693	PHE
3	B	1727	GLN
3	B	1729	LEU
3	B	1747	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	35	GLN
3	A	60	HIS
3	A	114	GLN
3	A	132	ASN

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Mol	Chain	Res	Type
3	A	173	HIS
3	A	232	GLN
3	A	239	GLN
3	A	269	GLN
3	A	357	GLN
3	A	415	HIS
3	A	468	GLN
3	A	585	ASN
3	A	595	GLN
3	A	685	HIS
3	A	696	HIS
3	B	1097	GLN
3	B	1114	GLN
3	B	1123	GLN
3	B	1173	HIS
3	B	1269	GLN
3	B	1289	GLN
3	B	1415	HIS
3	B	1474	GLN
3	B	1558	HIS
3	B	1585	ASN
3	B	1604	GLN
3	B	1685	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
4	SO4	A	852	-	4,4,4	0.25	0	6,6,6	0.09	0
5	BEF	B	1998	6	0,3,3	0.00	-	-		
6	ADP	B	1999	5	24,29,29	3.10	12 (50%)	29,45,45	2.39	6 (20%)
5	BEF	A	998	6	0,3,3	0.00	-	-		
6	ADP	A	999	5	24,29,29	3.41	12 (50%)	29,45,45	2.45	7 (24%)
4	SO4	B	1852	-	4,4,4	0.30	0	6,6,6	0.25	0
7	EDO	B	853	-	3,3,3	0.39	0	2,2,2	0.30	0

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
7	EDO	B	853	-	-	0/1/1/1	-
6	ADP	A	999	5	-	2/12/32/32	0/3/3/3
6	ADP	B	1999	5	-	0/12/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	999	ADP	C2-N3	7.96	1.44	1.32
6	A	999	ADP	C2-N1	7.88	1.48	1.33
6	B	1999	ADP	C2-N1	7.75	1.48	1.33
6	B	1999	ADP	C2-N3	7.05	1.43	1.32
6	A	999	ADP	C5'-C4'	5.60	1.69	1.51
6	B	1999	ADP	C5'-C4'	4.90	1.66	1.51
6	A	999	ADP	O4'-C1'	4.69	1.47	1.41
6	A	999	ADP	PB-O2B	-4.69	1.36	1.54
6	B	1999	ADP	O4'-C1'	3.86	1.46	1.41
6	A	999	ADP	C4-N3	3.81	1.40	1.35
6	A	999	ADP	C6-N6	-3.80	1.20	1.34
6	A	999	ADP	PA-O2A	-3.77	1.37	1.55
6	B	1999	ADP	C4-N3	3.75	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1999	ADP	C2'-C3'	-3.55	1.43	1.53
6	B	1999	ADP	PB-O2B	-3.52	1.41	1.54
6	B	1999	ADP	PA-O2A	-3.43	1.39	1.55
6	A	999	ADP	C2'-C3'	-3.28	1.44	1.53
6	B	1999	ADP	C6-N6	-3.21	1.22	1.34
6	A	999	ADP	C5-N7	-2.29	1.31	1.39
6	B	1999	ADP	C5-C4	2.23	1.46	1.40
6	B	1999	ADP	C5-N7	-2.17	1.31	1.39
6	B	1999	ADP	PB-O1B	-2.15	1.43	1.50
6	A	999	ADP	PB-O1B	-2.13	1.43	1.50
6	A	999	ADP	C5-C4	2.08	1.46	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	999	ADP	O3B-PB-O3A	8.24	132.27	104.64
6	B	1999	ADP	O3B-PB-O3A	7.90	131.13	104.64
6	B	1999	ADP	N3-C2-N1	-7.20	117.43	128.68
6	A	999	ADP	N3-C2-N1	-7.07	117.63	128.68
6	B	1999	ADP	O3A-PB-O1B	-3.37	92.50	111.19
6	A	999	ADP	O3A-PB-O1B	-3.33	92.72	111.19
6	A	999	ADP	C2'-C3'-C4'	2.96	108.40	102.64
6	B	1999	ADP	C2'-C3'-C4'	2.73	107.94	102.64
6	A	999	ADP	O2'-C2'-C1'	2.43	119.83	110.85
6	B	1999	ADP	O2'-C2'-C1'	2.38	119.63	110.85
6	B	1999	ADP	C2-N1-C6	2.32	122.71	118.75
6	A	999	ADP	O2A-PA-O1A	2.13	122.77	112.24
6	A	999	ADP	O2B-PB-O3A	-2.07	97.69	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	999	ADP	PA-O3A-PB-O3B
6	A	999	ADP	PA-O3A-PB-O1B

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	852	SO4	1	0

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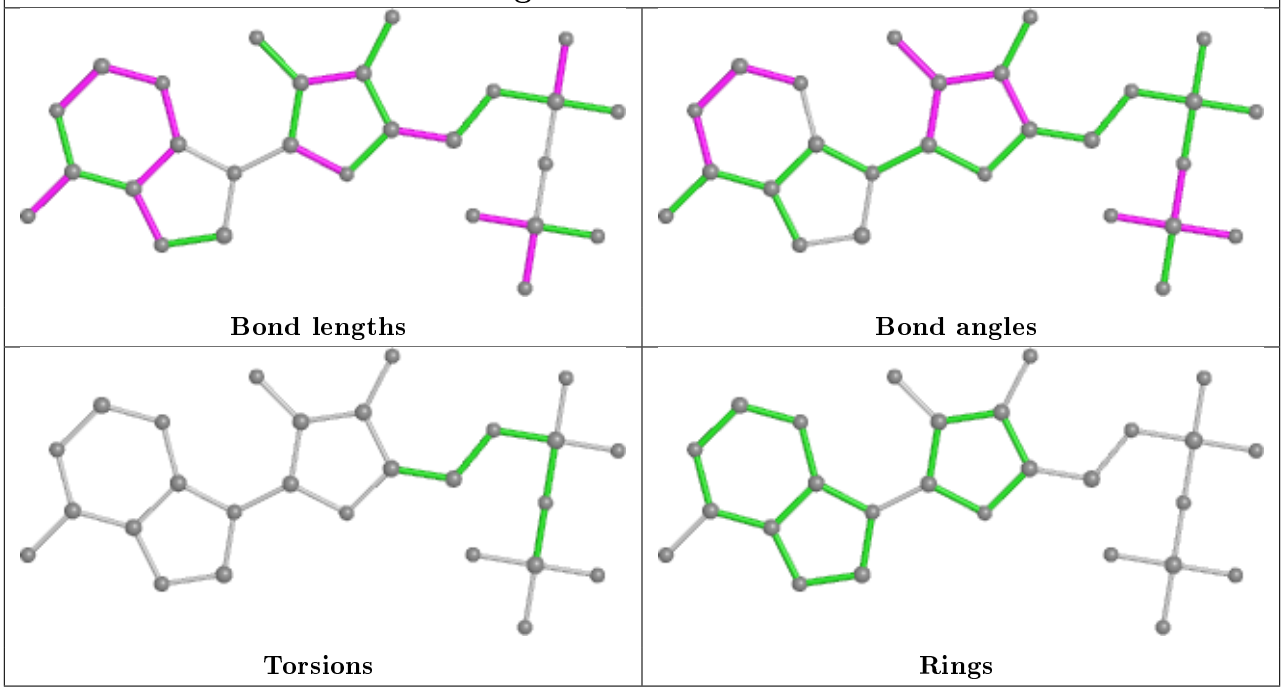
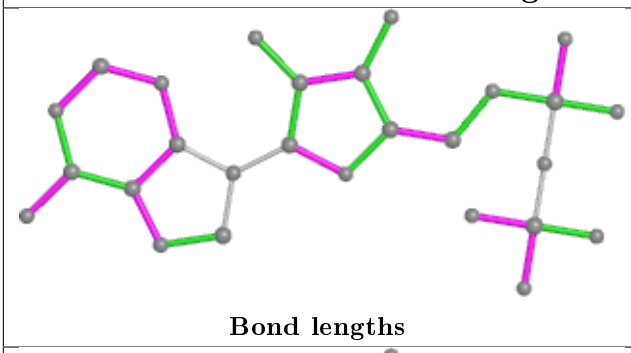
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1998	BEF	1	0
4	B	1852	SO4	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

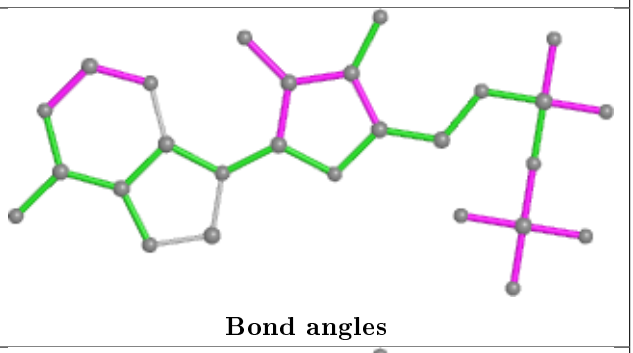
Ligand ADP B 1999



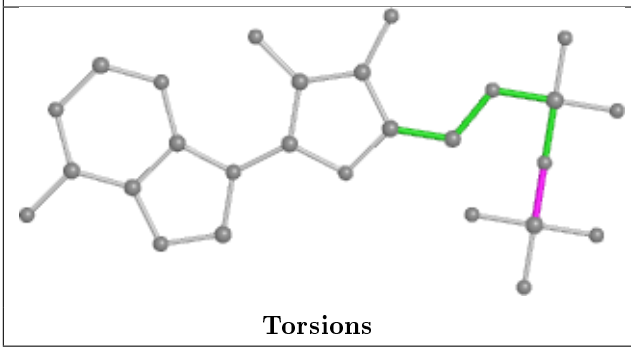
Ligand ADP A 999



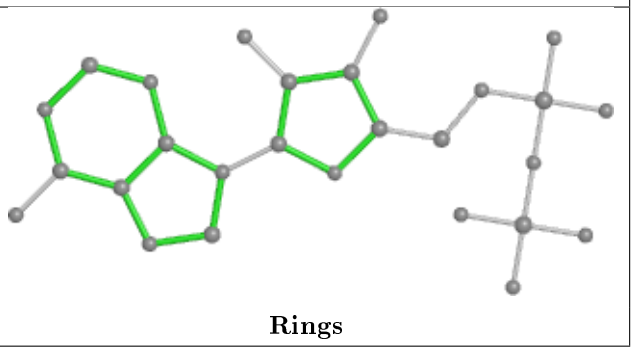
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	C	23/23 (100%)	0.87	2 (8%) 10 4	47, 84, 115, 146	0
2	D	22/22 (100%)	0.94	3 (13%) 3 1	60, 85, 156, 171	0
3	A	759/765 (99%)	-0.60	3 (0%) 92 85	3, 30, 81, 171	0
3	B	759/765 (99%)	-0.56	4 (0%) 91 82	3, 28, 101, 147	0
All	All	1563/1575 (99%)	-0.54	12 (0%) 86 74	3, 30, 97, 171	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1972	DG	4.9
3	A	1	MET	4.1
1	C	1901	DG	2.9
3	B	1393	LYS	2.8
3	A	635	GLY	2.7
3	B	1630	ASP	2.7
3	B	1462	LYS	2.6
2	D	1951	DG	2.4
2	D	1971	DC	2.4
3	B	1442	TYR	2.3
1	C	1916	DG	2.2
3	A	2	GLU	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

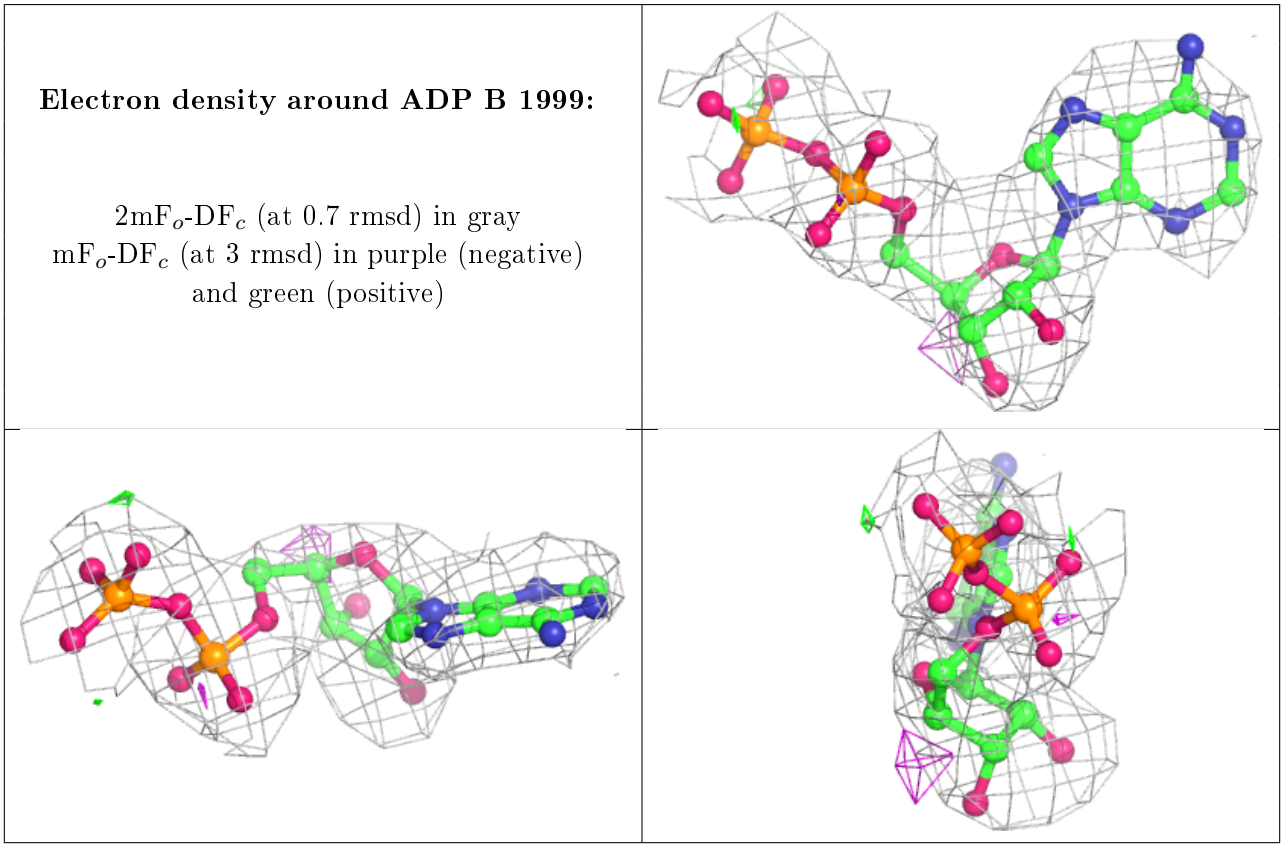
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	B	853	4/4	0.73	0.34	46,47,49,50	0
5	BEF	A	998	4/4	0.94	0.20	22,23,24,29	0
5	BEF	B	1998	4/4	0.95	0.14	18,19,21,25	0
6	ADP	B	1999	27/27	0.95	0.15	16,21,25,25	0
6	ADP	A	999	27/27	0.96	0.14	18,23,26,27	0
4	SO4	B	1852	5/5	0.97	0.14	34,34,36,36	0
4	SO4	A	852	5/5	0.98	0.14	38,39,40,41	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.

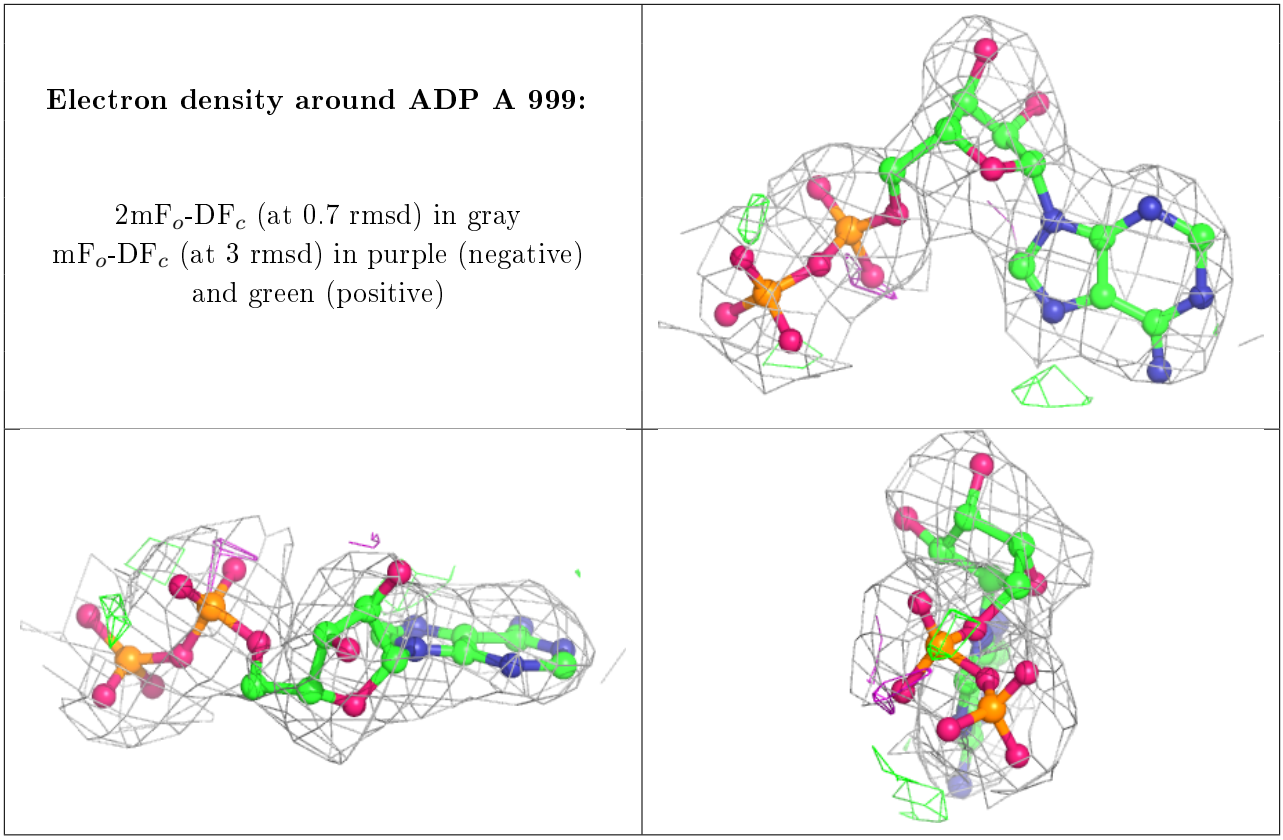
Electron density around ADP B 1999:

$2mF_o$-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 A 999:

$2mF_o$-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

There are no such residues in this entry.