



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:21 PM UTC

PDB ID : 2DFT / pdb\_00002dft  
Title : Structure of shikimate kinase from Mycobacterium tuberculosis complexed with ADP and Mg at 2.8 angstroms of resolution  
Authors : Dias, M.V.; Faim, L.M.; Vasconcelos, I.B.; de Oliveira, J.S.; Basso, L.A.; Santos, D.S.; de Azevedo, W.F.  
Deposited on : 2006-03-03  
Resolution : 2.80 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](mailto: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>.

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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

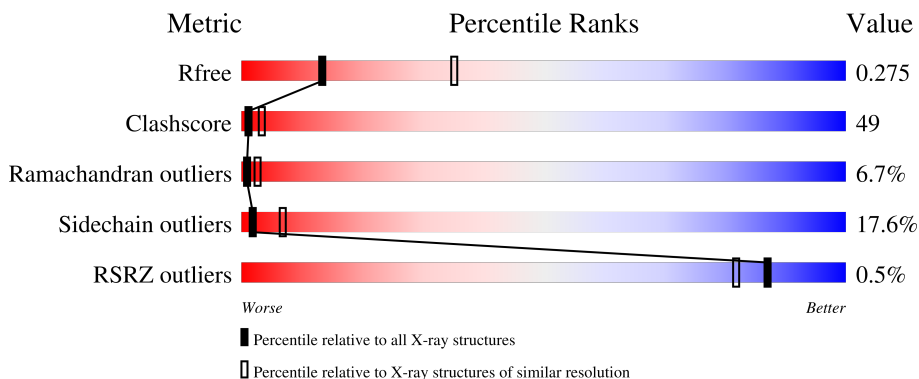
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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  $\geq 3$ , 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	176	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 10%; text-align: center;">%</div> <div style="width: 80%; position: relative; height: 15px;"> <div style="width: 24%; background-color: green;"></div> <div style="width: 38%; background-color: yellow;"></div> <div style="width: 21%; background-color: orange;"></div> <div style="width: 6%; background-color: red;"></div> <div style="width: 11%; background-color: grey;"></div> </div> <div style="width: 10%; text-align: center;">%</div> </div>
1	B	176	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 10%; text-align: center;">%</div> <div style="width: 80%; position: relative; height: 15px;"> <div style="width: 26%; background-color: green;"></div> <div style="width: 48%; background-color: yellow;"></div> <div style="width: 14%; background-color: orange;"></div> <div style="width: 6%; background-color: red;"></div> <div style="width: 6%; background-color: grey;"></div> </div> <div style="width: 10%; text-align: center;">%</div> </div>
1	C	176	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 10%; text-align: center;">%</div> <div style="width: 80%; position: relative; height: 15px;"> <div style="width: 20%; background-color: green;"></div> <div style="width: 37%; background-color: yellow;"></div> <div style="width: 24%; background-color: orange;"></div> <div style="width: 7%; background-color: red;"></div> <div style="width: 12%; background-color: grey;"></div> </div> <div style="width: 10%; text-align: center;">%</div> </div>
1	D	176	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 10%; text-align: center;">%</div> <div style="width: 80%; position: relative; height: 15px;"> <div style="width: 26%; background-color: green;"></div> <div style="width: 36%; background-color: yellow;"></div> <div style="width: 25%; background-color: orange;"></div> <div style="width: 6%; background-color: red;"></div> <div style="width: 6%; background-color: grey;"></div> </div> <div style="width: 10%; text-align: center;">%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5152 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 Shikimate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1165	717	232	214	2	0	0	0
1	B	165	1229	759	244	224	2	0	0	0
1	C	155	1157	713	230	212	2	0	0	0
1	D	165	1226	757	244	223	2	0	0	0

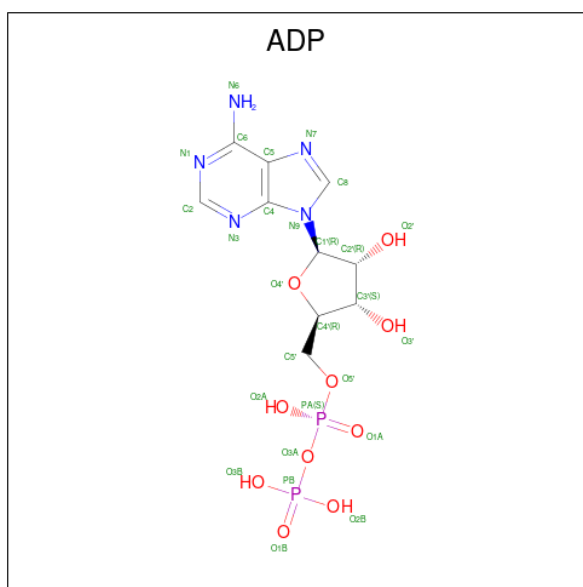
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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


- Molecule 5 is water.

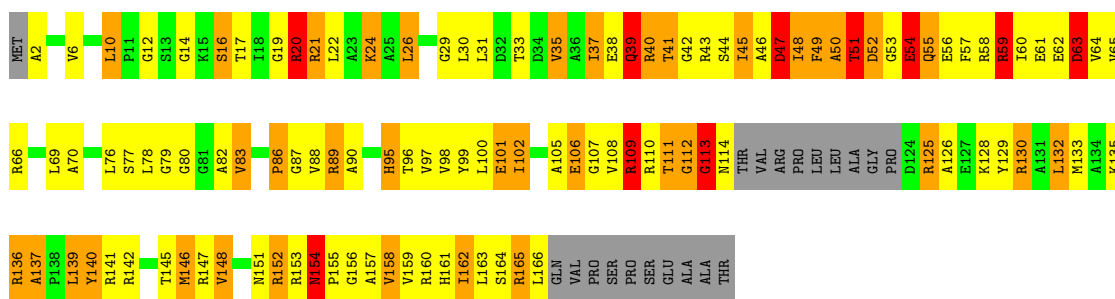
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		
5	B	85	Total	O	0	0
			85	85		
5	C	51	Total	O	0	0
			51	51		
5	D	64	Total	O	0	0
			64	64		

### 3 Residue-property plots

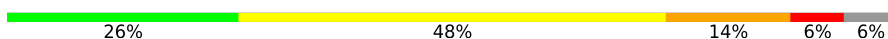
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

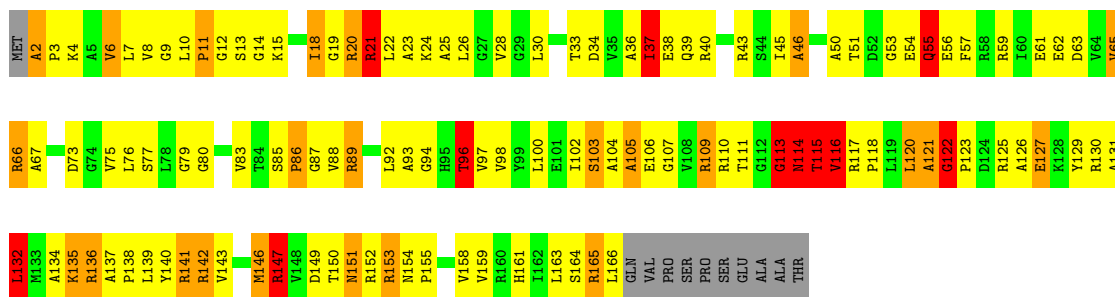
- Molecule 1: Shikimate kinase

Chain A: 




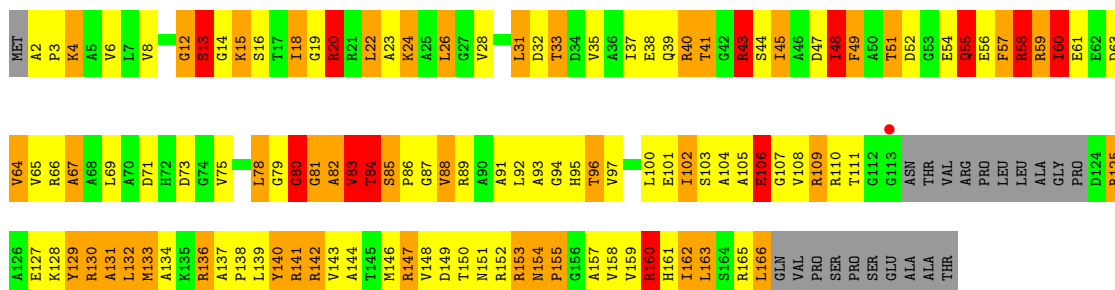
- Molecule 1: Shikimate kinase

Chain B: 

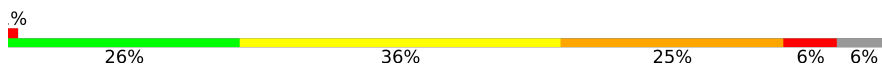


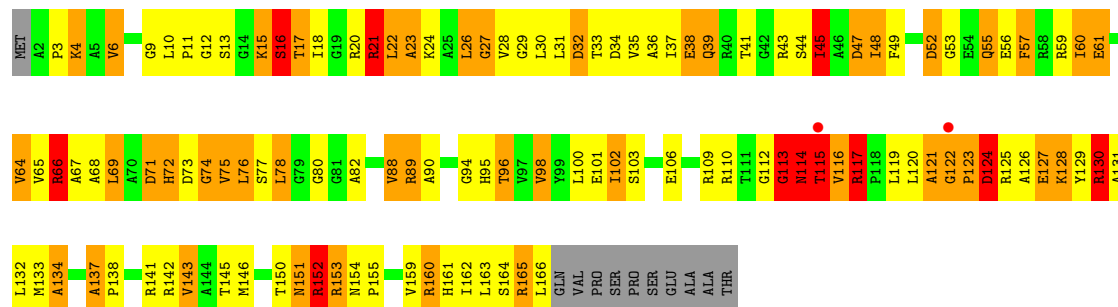
- Molecule 1: Shikimate kinase

Chain C: 



- Molecule 1: Shikimate kinase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.62Å 62.20Å 170.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.17 – 2.80 57.17 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (57.17-2.80) 99.7 (57.17-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.183 , 0.282 0.184 , 0.275	Depositor DCC
$R_{free}$ test set	832 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtrriage
Anisotropy	0.009	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.028 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, CL

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	1.68	8/1176 (0.7%)	2.43	78/1584 (4.9%)
1	B	1.62	8/1243 (0.6%)	2.23	52/1679 (3.1%)
1	C	1.75	14/1168 (1.2%)	2.41	65/1573 (4.1%)
1	D	1.71	11/1240 (0.9%)	2.36	69/1674 (4.1%)
All	All	1.69	41/4827 (0.8%)	2.36	264/6510 (4.1%)

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	A	0	3
1	B	0	4
1	C	0	4
1	D	0	6
All	All	0	17

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	VAL	CA-CB	-8.21	1.44	1.54
1	D	124	ASP	CA-C	7.70	1.63	1.52
1	A	83	VAL	CA-CB	-7.11	1.46	1.54
1	A	64	VAL	CA-CB	-7.08	1.44	1.54
1	C	91	ALA	CA-CB	-6.85	1.42	1.53
1	D	32	ASP	N-CA	6.49	1.54	1.46
1	D	114	ASN	CA-C	6.47	1.61	1.52
1	D	98	VAL	CA-CB	6.42	1.62	1.54
1	D	6	VAL	CA-CB	-6.40	1.46	1.54
1	C	111	THR	CA-C	6.38	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	49	PHE	N-CA	-6.35	1.38	1.46
1	C	18	ILE	C-O	6.15	1.31	1.24
1	D	49	PHE	C-O	-6.12	1.17	1.24
1	A	162	ILE	CA-CB	-6.08	1.46	1.54
1	C	94	GLY	N-CA	-6.02	1.39	1.45
1	D	45	ILE	CA-CB	-5.92	1.46	1.54
1	C	78	LEU	N-CA	-5.87	1.38	1.46
1	C	131	ALA	CA-CB	5.73	1.62	1.53
1	B	105	ALA	CA-CB	-5.70	1.43	1.53
1	C	60	ILE	CA-CB	5.62	1.60	1.54
1	C	80	GLY	C-O	5.60	1.31	1.23
1	C	84	THR	CB-CG2	5.57	1.71	1.52
1	C	144	ALA	C-O	-5.52	1.17	1.23
1	A	109	ARG	N-CA	-5.50	1.39	1.46
1	D	130	ARG	C-O	-5.38	1.17	1.24
1	A	113	GLY	N-CA	5.37	1.53	1.45
1	B	127	GLU	CA-C	-5.30	1.45	1.52
1	D	17	THR	CA-CB	5.30	1.61	1.53
1	D	53	GLY	N-CA	5.26	1.52	1.45
1	B	116	VAL	CA-CB	5.26	1.61	1.54
1	A	152	ARG	CA-C	5.25	1.59	1.52
1	B	97	VAL	CA-CB	-5.20	1.47	1.53
1	C	59	ARG	CB-CG	5.20	1.68	1.52
1	A	98	VAL	CA-CB	-5.17	1.48	1.54
1	C	48	ILE	CA-CB	5.13	1.61	1.54
1	B	39	GLN	C-O	-5.11	1.17	1.24
1	B	132	LEU	CA-C	5.10	1.59	1.52
1	B	36	ALA	CA-CB	-5.10	1.44	1.53
1	B	4	LYS	C-O	-5.09	1.18	1.24
1	C	67	ALA	N-CA	5.01	1.52	1.46
1	D	127	GLU	N-CA	5.01	1.52	1.46

All (264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	VAL	N-CA-C	12.90	122.80	110.42
1	C	83	VAL	N-CA-C	12.81	125.51	112.83
1	C	55	GLN	N-CA-C	-11.40	97.96	112.90
1	D	76	LEU	N-CA-C	-10.75	90.42	108.26
1	D	48	ILE	N-CA-C	-10.69	99.35	111.00
1	D	60	ILE	N-CA-C	-10.52	100.09	110.72
1	A	48	ILE	N-CA-C	-10.51	101.60	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	LEU	N-CA-C	-10.43	100.03	113.17
1	A	59	ARG	N-CA-C	-10.00	99.20	111.40
1	D	73	ASP	N-CA-C	-9.97	101.44	114.31
1	A	86	PRO	CA-C-N	9.94	131.01	119.98
1	A	86	PRO	C-N-CA	9.94	131.01	119.98
1	B	127	GLU	N-CA-C	-9.84	101.77	113.88
1	A	90	ALA	N-CA-C	-9.54	100.96	111.36
1	D	152	ARG	N-CA-C	-9.53	101.41	113.23
1	A	132	LEU	N-CA-C	-9.39	101.12	111.36
1	A	154	ASN	CA-C-N	-9.33	109.27	118.97
1	A	154	ASN	C-N-CA	-9.33	109.27	118.97
1	C	6	VAL	CA-C-O	-9.30	111.05	120.25
1	C	49	PHE	N-CA-C	-9.05	100.36	111.40
1	A	125	ARG	NE-CZ-NH1	-8.92	112.58	121.50
1	B	134	ALA	N-CA-C	-8.90	102.43	113.20
1	C	24	LYS	N-CA-C	-8.65	101.80	111.14
1	D	115	THR	N-CA-C	8.62	129.15	110.80
1	C	16	SER	N-CA-C	-8.56	100.96	111.40
1	C	143	VAL	CB-CA-C	-8.51	102.31	110.65
1	D	41	THR	N-CA-C	-8.49	102.71	113.23
1	A	51	THR	N-CA-C	8.44	124.50	114.04
1	C	139	LEU	N-CA-C	-8.44	101.31	111.69
1	A	20	ARG	N-CA-C	-8.36	102.16	111.28
1	A	39	GLN	CA-C-N	-8.35	110.05	122.24
1	A	39	GLN	C-N-CA	-8.35	110.05	122.24
1	A	163	LEU	N-CA-C	-8.33	101.44	111.69
1	D	153	ARG	N-CA-C	8.31	121.78	110.55
1	A	47	ASP	CA-C-N	-8.31	114.83	122.97
1	A	47	ASP	C-N-CA	-8.31	114.83	122.97
1	C	109	ARG	N-CA-C	-8.24	101.55	111.69
1	C	18	ILE	O-C-N	8.20	130.15	121.87
1	C	129	TYR	N-CA-C	-8.19	102.18	112.90
1	B	110	ARG	N-CA-C	-8.05	102.91	112.89
1	C	154	ASN	N-CA-C	-7.92	101.02	110.13
1	C	40	ARG	N-CA-C	7.83	119.90	111.36
1	D	64	VAL	N-CA-C	-7.78	101.36	111.09
1	A	148	VAL	CB-CA-C	-7.77	99.13	110.63
1	D	132	LEU	N-CA-C	-7.71	102.80	112.90
1	A	53	GLY	CA-C-O	-7.64	115.92	121.88
1	B	116	VAL	N-CA-CB	7.61	123.79	111.23
1	C	133	MET	N-CA-C	-7.50	102.80	110.97
1	D	117	ARG	CA-C-N	7.45	129.16	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ARG	C-N-CA	7.45	129.16	119.84
1	B	21	ARG	NE-CZ-NH1	-7.44	114.06	121.50
1	C	95	HIS	N-CA-C	-7.44	100.93	110.53
1	B	89	ARG	CA-C-O	7.41	128.63	120.63
1	C	88	VAL	N-CA-C	-7.40	102.93	111.00
1	B	9	GLY	CA-C-N	-7.32	109.71	121.57
1	B	9	GLY	C-N-CA	-7.32	109.71	121.57
1	C	33	THR	N-CA-C	7.30	119.24	111.28
1	A	70	ALA	N-CA-C	-7.23	101.63	112.04
1	A	164	SER	CA-CB-OG	-7.15	96.80	111.10
1	B	143	VAL	CB-CA-C	-7.14	101.92	110.84
1	A	64	VAL	N-CA-C	7.10	119.93	111.05
1	B	24	LYS	N-CA-CB	7.07	120.51	110.12
1	B	122	GLY	N-CA-C	7.02	126.67	112.34
1	B	96	THR	N-CA-C	-7.01	97.81	108.67
1	B	77	SER	CA-C-O	-6.85	113.41	120.54
1	D	18	ILE	N-CA-C	-6.85	102.26	111.44
1	D	36	ALA	N-CA-C	6.84	119.75	111.82
1	B	104	ALA	CA-C-N	-6.81	109.22	121.14
1	B	104	ALA	C-N-CA	-6.81	109.22	121.14
1	B	37	ILE	N-CA-C	6.81	117.56	110.62
1	D	6	VAL	N-CA-C	-6.78	98.67	108.17
1	A	97	VAL	N-CA-C	6.75	117.35	107.37
1	D	64	VAL	CA-C-N	-6.74	111.98	121.55
1	D	64	VAL	C-N-CA	-6.74	111.98	121.55
1	A	40	ARG	CB-CA-C	6.72	120.94	111.74
1	A	10	LEU	N-CA-C	6.71	119.17	109.84
1	D	3	PRO	CA-C-N	6.71	129.27	120.28
1	D	3	PRO	C-N-CA	6.71	129.27	120.28
1	A	137	ALA	CA-C-N	-6.70	113.30	120.47
1	A	137	ALA	C-N-CA	-6.70	113.30	120.47
1	C	160	ARG	NE-CZ-NH1	-6.68	114.82	121.50
1	D	61	GLU	N-CA-C	6.67	118.21	111.07
1	C	132	LEU	CA-CB-CG	6.67	139.64	116.30
1	B	102	ILE	CA-C-O	-6.66	113.78	120.90
1	B	109	ARG	N-CA-C	6.64	119.08	111.11
1	B	66	ARG	NE-CZ-NH1	-6.61	114.89	121.50
1	D	160	ARG	N-CA-C	6.59	118.16	110.97
1	A	140	TYR	N-CA-C	-6.58	104.18	111.36
1	C	20	ARG	NE-CZ-NH2	-6.54	113.31	119.20
1	D	154	ASN	CA-C-N	6.51	125.74	118.97
1	D	154	ASN	C-N-CA	6.51	125.74	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	SER	CA-C-O	6.46	124.43	119.46
1	A	37	ILE	CB-CA-C	-6.45	103.60	112.04
1	A	139	LEU	N-CA-C	6.44	119.12	111.71
1	B	104	ALA	N-CA-C	-6.44	104.31	111.71
1	D	66	ARG	N-CA-C	-6.43	104.32	111.71
1	D	96	THR	CA-C-N	-6.41	114.54	122.93
1	D	96	THR	C-N-CA	-6.41	114.54	122.93
1	D	124	ASP	N-CA-CB	-6.41	99.67	110.49
1	B	43	ARG	N-CA-C	6.36	119.49	110.14
1	C	59	ARG	N-CA-C	-6.35	104.23	112.23
1	B	4	LYS	CA-C-O	-6.35	113.59	121.02
1	C	48	ILE	N-CA-C	-6.34	96.16	109.34
1	A	20	ARG	NE-CZ-NH2	-6.32	113.52	119.20
1	A	26	LEU	N-CA-C	-6.31	104.46	111.71
1	A	164	SER	N-CA-C	6.27	118.92	111.71
1	D	34	ASP	N-CA-C	-6.27	103.75	111.40
1	D	142	ARG	CA-CB-CG	-6.23	101.64	114.10
1	B	2	ALA	CA-C-N	6.18	126.39	119.90
1	B	2	ALA	C-N-CA	6.18	126.39	119.90
1	C	43	ARG	O-C-N	-6.17	115.86	123.33
1	B	147	ARG	NE-CZ-NH1	-6.17	115.33	121.50
1	B	114	ASN	CA-C-N	6.16	133.31	121.54
1	B	114	ASN	C-N-CA	6.16	133.31	121.54
1	A	157	ALA	N-CA-C	6.15	119.63	111.75
1	B	164	SER	N-CA-C	-6.15	105.76	113.20
1	C	125	ARG	N-CA-C	6.11	120.74	113.28
1	D	88	VAL	N-CA-C	-6.11	104.68	110.42
1	D	17	THR	N-CA-CB	6.03	118.98	109.82
1	C	160	ARG	NE-CZ-NH2	5.98	124.59	119.20
1	A	106	GLU	N-CA-C	-5.98	104.84	111.36
1	B	19	GLY	N-CA-C	-5.95	105.60	112.50
1	B	67	ALA	N-CA-C	-5.94	104.81	111.28
1	D	151	ASN	N-CA-CB	5.94	118.58	109.91
1	A	79	GLY	N-CA-C	-5.94	104.41	111.36
1	B	66	ARG	CB-CA-C	-5.91	100.64	110.68
1	C	96	THR	CA-C-N	-5.90	115.41	123.14
1	C	96	THR	C-N-CA	-5.90	115.41	123.14
1	C	48	ILE	N-CA-CB	5.89	120.96	111.23
1	D	126	ALA	CA-C-O	-5.89	114.30	120.55
1	A	66	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	D	143	VAL	CA-C-N	-5.88	114.61	122.72
1	D	143	VAL	C-N-CA	-5.88	114.61	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	ARG	CB-CG-CD	5.86	124.79	111.30
1	D	21	ARG	NE-CZ-NH2	-5.86	113.93	119.20
1	D	38	GLU	N-CA-C	-5.85	104.98	111.36
1	C	82	ALA	N-CA-C	-5.84	106.00	113.01
1	D	133	MET	N-CA-C	5.83	117.31	111.07
1	B	103	SER	CA-CB-OG	-5.81	99.48	111.10
1	A	54	GLU	CA-C-N	5.81	128.86	120.79
1	A	54	GLU	C-N-CA	5.81	128.86	120.79
1	A	63	ASP	CB-CA-C	5.78	120.68	110.85
1	C	94	GLY	CA-C-O	-5.78	114.92	119.83
1	B	135	LYS	CB-CG-CD	5.78	124.58	111.30
1	A	66	ARG	CD-NE-CZ	-5.75	116.34	124.40
1	C	18	ILE	CB-CA-C	-5.75	103.25	112.16
1	A	146	MET	CA-C-N	-5.74	114.89	122.99
1	A	146	MET	C-N-CA	-5.74	114.89	122.99
1	A	100	LEU	CA-C-N	-5.74	113.60	122.09
1	A	100	LEU	C-N-CA	-5.74	113.60	122.09
1	A	142	ARG	N-CA-CB	5.73	119.16	110.28
1	D	128	LYS	CA-C-N	5.73	127.89	120.44
1	D	128	LYS	C-N-CA	5.73	127.89	120.44
1	C	163	LEU	CA-C-O	-5.71	113.65	120.10
1	C	13	SER	N-CA-C	-5.70	105.15	111.71
1	A	145	THR	N-CA-C	-5.66	105.58	112.88
1	B	11	PRO	CA-C-N	-5.65	113.63	122.51
1	B	11	PRO	C-N-CA	-5.65	113.63	122.51
1	A	80	GLY	CA-C-N	-5.65	113.71	122.30
1	A	80	GLY	C-N-CA	-5.65	113.71	122.30
1	A	65	VAL	N-CA-C	-5.64	104.40	112.35
1	B	19	GLY	CA-C-O	-5.64	114.91	121.00
1	B	134	ALA	CA-C-N	-5.63	111.94	121.18
1	B	134	ALA	C-N-CA	-5.63	111.94	121.18
1	D	55	GLN	N-CA-CB	5.60	118.91	109.78
1	D	72	HIS	N-CA-C	-5.58	100.60	109.59
1	B	83	VAL	CA-C-O	-5.58	113.81	120.78
1	A	111	THR	N-CA-C	5.57	119.80	112.89
1	D	26	LEU	CB-CA-C	-5.55	102.19	111.13
1	D	9	GLY	N-CA-C	-5.55	102.50	110.38
1	C	43	ARG	NE-CZ-NH2	-5.55	114.21	119.20
1	C	111	THR	CB-CA-C	5.54	121.45	110.42
1	C	147	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	D	16	SER	CA-C-O	-5.53	114.64	120.55
1	A	165	ARG	CB-CA-C	5.51	120.59	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	PRO	O-C-N	5.50	130.06	122.64
1	B	93	ALA	CA-C-N	-5.50	115.66	123.08
1	B	93	ALA	C-N-CA	-5.50	115.66	123.08
1	D	134	ALA	CA-C-N	-5.46	111.59	120.72
1	D	134	ALA	C-N-CA	-5.46	111.59	120.72
1	A	26	LEU	CB-CA-C	-5.46	100.52	110.63
1	A	42	GLY	N-CA-C	-5.45	106.49	114.61
1	C	41	THR	N-CA-CB	-5.45	102.61	110.56
1	D	20	ARG	N-CA-CB	5.44	118.22	110.16
1	A	47	ASP	N-CA-C	5.41	122.32	110.80
1	B	132	LEU	CD1-CG-CD2	5.41	122.70	110.80
1	A	77	SER	CB-CA-C	-5.37	101.49	110.19
1	A	96	THR	CB-CA-C	-5.36	101.97	110.81
1	C	136	ARG	CG-CD-NE	-5.35	100.23	112.00
1	D	109	ARG	N-CA-C	-5.35	106.26	112.89
1	B	158	VAL	N-CA-C	-5.33	105.19	111.00
1	C	101	GLU	CA-C-N	-5.33	115.53	122.51
1	C	101	GLU	C-N-CA	-5.33	115.53	122.51
1	C	58	ARG	CA-C-N	-5.31	111.65	120.68
1	C	58	ARG	C-N-CA	-5.31	111.65	120.68
1	D	75	VAL	CB-CA-C	-5.29	102.75	110.62
1	A	158	VAL	N-CA-C	-5.28	105.38	110.72
1	A	70	ALA	CA-C-N	-5.25	113.21	123.13
1	A	70	ALA	C-N-CA	-5.25	113.21	123.13
1	C	84	THR	N-CA-C	5.25	118.47	111.75
1	C	136	ARG	O-C-N	5.25	128.12	122.34
1	A	88	VAL	CB-CA-C	-5.25	104.98	112.22
1	D	77	SER	CB-CA-C	5.25	118.80	110.19
1	A	160	ARG	CA-CB-CG	-5.22	103.66	114.10
1	B	65	VAL	CB-CA-C	-5.22	105.29	111.97
1	A	95	HIS	N-CA-C	5.21	116.82	110.41
1	D	30	LEU	CA-C-O	-5.21	115.27	121.16
1	D	130	ARG	N-CA-C	-5.20	105.73	111.71
1	D	71	ASP	N-CA-C	5.20	120.76	113.02
1	C	4	LYS	CD-CE-NZ	-5.18	95.31	111.90
1	C	60	ILE	CG1-CB-CG2	-5.18	95.16	110.70
1	A	148	VAL	CA-C-N	-5.18	114.89	122.19
1	A	148	VAL	C-N-CA	-5.18	114.89	122.19
1	A	163	LEU	CB-CA-C	-5.18	101.23	110.70
1	C	95	HIS	N-CA-CB	5.18	117.84	110.44
1	A	109	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	C	12	GLY	CA-C-N	-5.17	112.83	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	GLY	C-N-CA	-5.17	112.83	120.28
1	C	111	THR	N-CA-C	5.17	121.82	110.80
1	C	97	VAL	CA-C-N	-5.17	116.42	122.93
1	C	97	VAL	C-N-CA	-5.17	116.42	122.93
1	B	8	VAL	CA-C-O	-5.16	116.40	121.67
1	D	130	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	A	2	ALA	CA-C-N	-5.16	114.46	119.78
1	A	2	ALA	C-N-CA	-5.16	114.46	119.78
1	B	116	VAL	CA-CB-CG2	5.16	119.17	110.40
1	B	146	MET	CB-CG-SD	-5.15	97.24	112.70
1	D	38	GLU	CG-CD-OE1	-5.13	106.59	118.40
1	A	6	VAL	N-CA-CB	-5.13	105.44	111.90
1	A	63	ASP	N-CA-C	-5.13	105.77	111.36
1	B	12	GLY	N-CA-C	5.13	121.59	114.92
1	C	75	VAL	CB-CA-C	-5.12	104.04	111.68
1	D	20	ARG	N-CA-C	-5.12	105.78	111.36
1	A	21	ARG	CB-CG-CD	5.12	123.07	111.30
1	A	35	VAL	N-CA-CB	5.11	118.25	110.58
1	B	6	VAL	N-CA-CB	-5.11	105.23	111.67
1	C	64	VAL	CB-CA-C	-5.11	105.43	111.97
1	A	16	SER	CA-C-O	5.11	125.91	120.24
1	D	31	LEU	CA-C-O	-5.10	114.84	120.30
1	D	78	LEU	CB-CG-CD2	-5.10	95.40	110.70
1	D	29	GLY	CA-C-N	-5.08	114.69	122.87
1	D	29	GLY	C-N-CA	-5.08	114.69	122.87
1	C	162	ILE	CA-C-N	-5.08	112.97	120.28
1	C	162	ILE	C-N-CA	-5.08	112.97	120.28
1	C	93	ALA	CA-C-N	-5.07	117.92	123.30
1	C	93	ALA	C-N-CA	-5.07	117.92	123.30
1	A	95	HIS	CA-C-N	-5.06	115.69	122.42
1	A	95	HIS	C-N-CA	-5.06	115.69	122.42
1	C	140	TYR	N-CA-C	-5.06	105.85	111.36
1	C	141	ARG	N-CA-C	-5.05	107.18	113.19
1	D	57	PHE	CB-CA-C	-5.05	102.95	110.88
1	D	128	LYS	CD-CE-NZ	-5.05	95.75	111.90
1	B	96	THR	OG1-CB-CG2	-5.04	99.23	109.30
1	D	124	ASP	O-C-N	-5.04	115.89	122.59
1	C	106	GLU	CB-CG-CD	5.03	121.15	112.60
1	D	6	VAL	CB-CA-C	-5.03	103.33	110.83
1	C	22	LEU	CA-C-O	5.03	125.75	119.97
1	D	137	ALA	CA-C-N	5.03	124.63	119.05
1	D	137	ALA	C-N-CA	5.03	124.63	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	LEU	CA-C-N	-5.01	110.79	121.32
1	D	100	LEU	C-N-CA	-5.01	110.79	121.32
1	A	21	ARG	CA-CB-CG	-5.01	104.09	114.10
1	C	106	GLU	N-CA-C	5.01	116.59	111.03
1	A	159	VAL	N-CA-CB	5.00	116.40	110.55

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Mainchain
1	A	111	THR	Peptide
1	A	113	GLY	Peptide
1	B	113	GLY	Peptide
1	B	114	ASN	Peptide
1	B	115	THR	Peptide
1	B	120	LEU	Peptide
1	C	106	GLU	Peptide
1	C	13	SER	Mainchain
1	C	73	ASP	Mainchain
1	C	83	VAL	Peptide
1	D	113	GLY	Peptide
1	D	114	ASN	Peptide
1	D	115	THR	Peptide
1	D	124	ASP	Peptide
1	D	23	ALA	Peptide
1	D	94	GLY	Peptide

## 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	A	1165	0	1208	116	0
1	B	1229	0	1282	118	1
1	C	1157	0	1202	130	1
1	D	1226	0	1275	119	1
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	27	0	12	6	0
4	B	27	0	12	2	0
4	C	27	0	12	8	0
4	D	27	0	12	6	0
5	A	60	0	0	32	2
5	B	85	0	0	47	1
5	C	51	0	0	40	1
5	D	64	0	0	34	1
All	All	5152	0	5015	482	4

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 49.

All (482) 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:165:ARG:HH11	1:B:165:ARG:CG	1.34	1.37
1:A:59:ARG:HB2	5:A:278:HOH:O	1.15	1.31
1:C:157:ALA:HB3	5:C:411:HOH:O	1.25	1.29
1:A:125:ARG:HA	5:A:387:HOH:O	1.21	1.28
1:B:116:VAL:CG1	5:B:373:HOH:O	1.66	1.25
1:B:116:VAL:HG12	5:B:373:HOH:O	1.25	1.22
1:D:11:PRO:HG2	5:D:353:HOH:O	1.40	1.20
1:D:121:ALA:C	1:D:123:PRO:HD2	1.66	1.19
4:A:180:ADP:O2A	5:A:449:HOH:O	1.61	1.16
1:A:24:LYS:HE2	5:A:303:HOH:O	1.44	1.15
1:C:157:ALA:CB	5:C:411:HOH:O	1.80	1.13
1:D:113:GLY:HA3	5:D:344:HOH:O	1.49	1.12
1:C:160:ARG:HD3	5:C:345:HOH:O	1.49	1.11
1:A:86:PRO:HA	5:A:379:HOH:O	1.48	1.10
1:A:113:GLY:HA3	5:A:315:HOH:O	1.47	1.10
1:D:116:VAL:HA	5:D:336:HOH:O	1.52	1.10
1:A:152:ARG:HG3	5:A:268:HOH:O	1.53	1.08
1:C:44:SER:HB3	5:C:277:HOH:O	0.92	1.07
1:A:51:THR:HG22	1:A:52:ASP:OD2	1.56	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HG	5:B:442:HOH:O	1.56	1.06
1:D:165:ARG:HG2	1:D:165:ARG:NH1	1.55	1.05
1:B:121:ALA:HB3	5:B:400:HOH:O	1.56	1.04
1:A:63:ASP:HB3	5:A:383:HOH:O	1.58	1.04
1:A:152:ARG:HA	5:A:299:HOH:O	0.87	1.04
1:B:165:ARG:HH11	1:B:165:ARG:HG3	0.91	1.04
1:D:165:ARG:HH11	1:D:165:ARG:CG	1.72	1.02
1:B:165:ARG:CG	1:B:165:ARG:NH1	2.09	1.02
1:D:16:SER:HB3	1:D:32:ASP:OD2	1.57	1.02
1:C:40:ARG:HD3	5:C:316:HOH:O	1.57	1.01
1:C:55:GLN:HG3	5:C:221:HOH:O	1.58	1.01
1:C:130:ARG:HG3	1:C:130:ARG:HH11	1.26	0.99
1:D:13:SER:N	5:D:407:HOH:O	1.94	0.99
1:D:163:LEU:HD23	5:D:396:HOH:O	1.63	0.99
1:C:108:VAL:HA	5:C:413:HOH:O	1.62	0.97
1:D:47:ASP:HB2	5:D:226:HOH:O	1.65	0.96
1:A:10:LEU:HD11	1:A:133:MET:HG3	1.48	0.95
1:B:127:GLU:HB3	5:B:358:HOH:O	1.67	0.95
1:B:165:ARG:HG3	1:B:165:ARG:NH1	1.71	0.94
1:D:121:ALA:O	1:D:123:PRO:HG2	1.67	0.94
1:A:102:ILE:HD12	1:A:151:ASN:OD1	1.66	0.94
1:C:130:ARG:HH11	1:C:130:ARG:CG	1.79	0.94
1:D:15:LYS:HG2	4:D:183:ADP:O1B	1.69	0.93
5:B:447:HOH:O	1:C:24:LYS:CD	2.17	0.92
1:C:105:ALA:N	5:C:463:HOH:O	2.01	0.92
1:A:141:ARG:HD2	1:A:147:ARG:HH21	1.30	0.92
1:B:130:ARG:HD2	5:B:369:HOH:O	1.69	0.92
1:C:2:ALA:HB1	1:C:3:PRO:HD2	1.50	0.91
1:B:121:ALA:CB	5:B:400:HOH:O	2.10	0.91
1:B:165:ARG:HH11	1:B:165:ARG:HG2	1.36	0.90
1:C:160:ARG:HH11	1:C:160:ARG:HG2	1.35	0.90
1:C:81:GLY:N	5:C:331:HOH:O	2.06	0.88
1:A:20:ARG:HD2	5:B:293:HOH:O	1.74	0.87
1:A:114:ASN:ND2	5:A:314:HOH:O	2.06	0.87
1:C:41:THR:O	1:C:43:ARG:HG2	1.73	0.87
1:B:113:GLY:HA2	5:B:271:HOH:O	1.73	0.87
1:D:12:GLY:N	5:D:407:HOH:O	2.08	0.86
1:D:121:ALA:C	1:D:123:PRO:CD	2.47	0.85
1:C:40:ARG:CD	5:C:316:HOH:O	2.17	0.84
5:B:447:HOH:O	1:C:24:LYS:HD3	1.75	0.84
1:B:121:ALA:C	5:B:401:HOH:O	2.21	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ASN:HA	5:C:445:HOH:O	1.78	0.83
1:C:104:ALA:O	1:C:108:VAL:HG23	1.78	0.83
1:C:152:ARG:HD3	5:C:430:HOH:O	1.79	0.83
1:D:102:ILE:HD11	1:D:106:GLU:HB3	1.60	0.83
1:A:86:PRO:CA	5:A:379:HOH:O	2.10	0.82
1:B:33:THR:O	1:B:37:ILE:HG13	1.79	0.82
1:A:89:ARG:HG3	1:A:89:ARG:HH11	1.42	0.81
1:A:136:ARG:HG2	1:A:136:ARG:HH11	1.47	0.80
1:A:10:LEU:CD1	1:A:133:MET:HG3	2.11	0.79
1:B:122:GLY:N	5:B:401:HOH:O	2.15	0.79
1:C:2:ALA:HB1	1:C:3:PRO:CD	2.11	0.79
1:D:131:ALA:HB1	5:D:395:HOH:O	1.82	0.79
1:D:113:GLY:CA	5:D:344:HOH:O	2.17	0.79
1:D:164:SER:HB2	1:D:165:ARG:HH12	1.46	0.79
1:A:106:GLU:HG2	5:A:425:HOH:O	1.82	0.78
1:B:50:ALA:HA	1:D:122:GLY:O	1.83	0.78
1:B:127:GLU:HG2	5:B:362:HOH:O	1.84	0.78
1:C:51:THR:HG22	5:C:274:HOH:O	1.82	0.78
1:A:136:ARG:HH11	1:A:136:ARG:CG	1.94	0.78
1:C:15:LYS:HG3	4:C:182:ADP:O1B	1.83	0.77
1:C:149:ASP:OD1	1:C:151:ASN:HB2	1.84	0.77
1:A:146:MET:SD	5:A:243:HOH:O	2.42	0.77
1:C:152:ARG:HG2	5:C:462:HOH:O	1.83	0.77
1:D:102:ILE:CD1	1:D:106:GLU:HB3	2.15	0.77
1:B:94:GLY:O	5:B:310:HOH:O	2.02	0.76
1:B:147:ARG:O	1:B:147:ARG:HG3	1.85	0.76
1:C:150:THR:HG22	1:C:158:VAL:HG21	1.65	0.76
1:A:141:ARG:CD	1:A:147:ARG:HH21	1.98	0.76
1:C:141:ARG:HD2	1:C:147:ARG:NH2	2.01	0.76
1:D:23:ALA:HB2	1:D:75:VAL:HG21	1.68	0.76
1:B:121:ALA:HB1	5:B:401:HOH:O	1.85	0.75
1:D:122:GLY:N	1:D:123:PRO:HD2	2.00	0.75
1:C:152:ARG:HD2	5:C:462:HOH:O	1.87	0.75
1:D:165:ARG:HG2	1:D:165:ARG:HH11	0.76	0.75
1:B:61:GLU:O	1:B:65:VAL:HG23	1.87	0.75
1:A:86:PRO:HG2	1:A:87:GLY:H	1.52	0.74
1:D:35:VAL:HG12	1:D:39:GLN:NE2	2.03	0.74
1:B:51:THR:HA	5:B:472:HOH:O	1.86	0.74
1:C:152:ARG:CD	5:C:462:HOH:O	2.35	0.74
1:D:117:ARG:HG2	5:D:242:HOH:O	1.86	0.73
1:A:55:GLN:H	1:A:55:GLN:CD	1.97	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:HB2	5:A:425:HOH:O	1.86	0.73
1:C:67:ALA:O	1:C:71:ASP:HB2	1.88	0.72
4:A:180:ADP:O3'	4:B:181:ADP:O3'	2.07	0.72
1:B:165:ARG:NH1	1:B:165:ARG:HG2	1.93	0.72
1:C:130:ARG:HG3	1:C:130:ARG:NH1	2.03	0.72
4:C:182:ADP:O3'	4:D:183:ADP:O2'	2.07	0.72
1:D:38:GLU:OE2	5:D:326:HOH:O	2.08	0.72
1:A:102:ILE:CD1	1:A:151:ASN:HA	2.20	0.71
1:D:129:TYR:CD1	1:D:129:TYR:C	2.66	0.71
1:A:99:TYR:HD2	1:A:147:ARG:HG2	1.55	0.71
1:C:83:VAL:O	1:C:89:ARG:NH1	2.24	0.71
1:C:152:ARG:CG	5:C:462:HOH:O	2.39	0.70
1:C:51:THR:C	5:C:274:HOH:O	2.33	0.70
1:D:164:SER:HB2	1:D:165:ARG:NH1	2.06	0.70
1:C:160:ARG:HG2	1:C:160:ARG:NH1	2.05	0.69
1:C:8:VAL:HG12	1:C:78:LEU:HD22	1.75	0.69
1:D:114:ASN:HB2	5:D:319:HOH:O	1.90	0.69
1:B:116:VAL:N	5:B:215:HOH:O	2.20	0.69
1:B:153:ARG:HH21	1:B:161:HIS:CG	2.09	0.69
1:A:43:ARG:CG	5:A:323:HOH:O	2.41	0.69
1:C:133:MET:HG3	5:C:421:HOH:O	1.91	0.69
1:B:141:ARG:NH1	5:B:304:HOH:O	2.26	0.69
1:D:4:LYS:HB2	1:D:74:GLY:O	1.93	0.69
1:A:69:LEU:HD22	1:A:95:HIS:CE1	2.28	0.68
1:A:69:LEU:HD22	1:A:95:HIS:NE2	2.08	0.68
1:B:154:ASN:HB2	1:B:155:PRO:HD3	1.75	0.68
1:D:155:PRO:O	1:D:159:VAL:HG23	1.93	0.68
1:A:128:LYS:HG2	1:C:43:ARG:CZ	2.23	0.68
1:B:121:ALA:HB1	1:D:123:PRO:HG3	1.75	0.68
4:C:182:ADP:N7	5:C:220:HOH:O	2.25	0.68
1:A:37:ILE:O	1:A:41:THR:HG23	1.93	0.68
1:A:43:ARG:HG2	5:A:323:HOH:O	1.93	0.68
1:C:84:THR:HG21	5:C:456:HOH:O	1.93	0.68
1:A:106:GLU:CB	5:A:425:HOH:O	2.42	0.68
1:D:121:ALA:O	1:D:123:PRO:CG	2.41	0.67
1:B:11:PRO:HD3	5:B:229:HOH:O	1.95	0.67
1:A:89:ARG:NH2	5:A:378:HOH:O	2.26	0.67
1:B:2:ALA:O	1:B:73:ASP:HA	1.95	0.67
1:D:56:GLU:OE1	5:D:354:HOH:O	2.14	0.66
1:B:80:GLY:N	5:B:227:HOH:O	2.27	0.66
1:D:23:ALA:HB2	1:D:75:VAL:CG2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:HG3	1:A:89:ARG:NH1	2.04	0.66
1:A:106:GLU:CG	5:A:425:HOH:O	2.41	0.66
1:A:105:ALA:O	1:A:109:ARG:HD3	1.95	0.66
1:B:154:ASN:HB2	1:B:155:PRO:CD	2.26	0.66
1:A:141:ARG:HD3	5:A:294:HOH:O	1.96	0.66
1:A:17:THR:N	5:A:449:HOH:O	2.02	0.65
1:B:146:MET:HG3	5:B:422:HOH:O	1.96	0.65
1:C:130:ARG:CG	1:C:130:ARG:NH1	2.51	0.65
1:C:37:ILE:HG12	1:C:64:VAL:HG21	1.78	0.65
1:B:137:ALA:N	1:B:138:PRO:CD	2.60	0.64
1:C:47:ASP:O	1:C:48:ILE:HG13	1.97	0.64
1:C:80:GLY:CA	5:C:331:HOH:O	2.44	0.64
1:D:138:PRO:HG2	5:D:239:HOH:O	1.97	0.64
1:A:89:ARG:HH11	1:A:89:ARG:CG	2.12	0.63
1:A:128:LYS:HE2	1:C:52:ASP:OD1	1.98	0.63
1:D:88:VAL:O	1:D:89:ARG:C	2.39	0.63
1:D:17:THR:O	1:D:21:ARG:HG3	1.99	0.63
1:D:161:HIS:C	1:D:161:HIS:CD2	2.75	0.63
1:C:55:GLN:CG	5:C:221:HOH:O	2.27	0.63
1:B:122:GLY:CA	5:B:401:HOH:O	2.47	0.63
1:B:137:ALA:N	1:B:138:PRO:HD2	2.14	0.62
1:D:47:ASP:CB	5:D:226:HOH:O	2.35	0.62
1:D:129:TYR:CE2	5:D:353:HOH:O	2.51	0.62
1:D:22:LEU:HA	1:D:159:VAL:HG13	1.81	0.62
1:A:47:ASP:O	1:A:51:THR:HB	1.99	0.62
1:A:24:LYS:CE	5:A:303:HOH:O	2.21	0.62
1:C:88:VAL:O	1:C:92:LEU:HG	2.00	0.62
1:D:151:ASN:HB3	5:D:240:HOH:O	2.00	0.61
1:C:58:ARG:NH1	1:C:61:GLU:OE1	2.33	0.61
1:C:130:ARG:O	1:C:133:MET:HB3	2.01	0.61
1:B:116:VAL:HG23	1:B:117:ARG:H	1.64	0.61
1:A:101:GLU:OE2	1:A:147:ARG:HD3	2.01	0.61
1:B:89:ARG:HD2	1:B:142:ARG:NH2	2.16	0.61
1:C:52:ASP:HB3	5:C:392:HOH:O	2.01	0.61
1:C:52:ASP:O	1:C:56:GLU:HB3	2.01	0.60
1:C:127:GLU:HA	1:C:130:ARG:HB2	1.84	0.60
1:A:99:TYR:CD2	1:A:147:ARG:HG2	2.36	0.60
1:C:31:LEU:HD23	1:C:32:ASP:H	1.65	0.60
1:C:141:ARG:HD2	1:C:147:ARG:HH22	1.66	0.60
1:B:57:PHE:C	1:B:57:PHE:CD2	2.80	0.60
1:D:106:GLU:O	1:D:110:ARG:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:182:ADP:O3'	4:D:183:ADP:O3'	2.07	0.60
1:D:120:LEU:O	1:D:121:ALA:C	2.45	0.60
1:D:134:ALA:O	5:D:239:HOH:O	2.17	0.59
1:A:114:ASN:C	5:A:423:HOH:O	2.45	0.59
1:D:102:ILE:HD11	1:D:106:GLU:CB	2.31	0.59
1:D:112:GLY:C	1:D:114:ASN:N	2.61	0.59
1:D:72:HIS:NE2	1:D:74:GLY:HA3	2.18	0.59
1:C:165:ARG:O	1:C:166:LEU:C	2.46	0.59
1:B:113:GLY:O	1:B:114:ASN:HB2	2.02	0.58
1:C:13:SER:HB3	1:C:100:LEU:HB2	1.85	0.58
1:A:86:PRO:CG	1:A:87:GLY:H	2.15	0.58
1:A:99:TYR:CD1	1:A:140:TYR:HB3	2.39	0.58
1:B:121:ALA:CB	5:B:401:HOH:O	2.49	0.58
1:D:98:VAL:HG11	1:D:162:ILE:HG12	1.85	0.58
1:C:58:ARG:HH11	1:C:58:ARG:HG2	1.69	0.58
1:C:141:ARG:CG	5:C:420:HOH:O	2.50	0.58
1:B:117:ARG:HG2	1:B:117:ARG:HH11	1.69	0.58
1:A:10:LEU:HD11	1:A:133:MET:CG	2.29	0.57
1:A:33:THR:O	1:A:37:ILE:HG13	2.05	0.57
1:B:50:ALA:O	5:B:472:HOH:O	2.17	0.57
5:B:374:HOH:O	1:C:28:VAL:HA	2.03	0.57
1:D:138:PRO:CG	5:D:239:HOH:O	2.52	0.57
1:C:148:VAL:HG22	1:C:161:HIS:HD2	1.70	0.57
1:B:79:GLY:C	5:B:227:HOH:O	2.47	0.57
1:A:31:LEU:O	1:A:76:LEU:HD12	2.04	0.57
1:C:137:ALA:O	1:C:141:ARG:HG3	2.04	0.57
1:C:160:ARG:CD	5:C:345:HOH:O	2.27	0.57
1:C:18:ILE:HG22	1:C:18:ILE:O	2.04	0.56
1:D:35:VAL:HG12	1:D:39:GLN:HE21	1.66	0.56
1:D:96:THR:CG2	1:D:146:MET:HE3	2.35	0.56
1:A:46:ALA:O	1:A:48:ILE:N	2.38	0.56
1:B:150:THR:O	1:B:151:ASN:C	2.48	0.56
1:D:45:ILE:HD13	1:D:57:PHE:CE1	2.41	0.56
1:A:29:GLY:N	5:A:397:HOH:O	2.32	0.56
1:A:45:ILE:HG12	1:A:57:PHE:HE1	1.70	0.56
1:A:14:GLY:HA2	4:A:180:ADP:O2A	2.05	0.56
1:D:129:TYR:C	1:D:129:TYR:HD1	2.14	0.56
1:C:152:ARG:NH1	5:C:462:HOH:O	2.13	0.56
1:B:136:ARG:HA	5:B:442:HOH:O	2.05	0.55
1:A:35:VAL:O	1:A:39:GLN:HB2	2.06	0.55
1:B:117:ARG:HG2	1:B:117:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ALA:N	1:D:138:PRO:CD	2.69	0.55
1:A:141:ARG:CG	1:A:147:ARG:HH21	2.19	0.55
1:B:130:ARG:HB3	5:B:361:HOH:O	2.05	0.55
1:C:79:GLY:O	1:C:80:GLY:C	2.50	0.55
1:D:26:LEU:O	1:D:27:GLY:C	2.49	0.55
1:D:17:THR:OG1	4:D:183:ADP:H2'	2.07	0.55
4:A:180:ADP:HO2'	4:B:181:ADP:HO3'	1.55	0.54
1:B:116:VAL:HG11	5:B:373:HOH:O	1.67	0.54
1:D:89:ARG:HG2	1:D:143:VAL:HG11	1.89	0.54
1:A:155:PRO:O	1:A:156:GLY:C	2.50	0.54
1:B:22:LEU:HD23	1:B:75:VAL:CG2	2.38	0.54
4:D:183:ADP:PB	5:D:407:HOH:O	2.66	0.54
1:A:56:GLU:HG2	5:A:384:HOH:O	2.08	0.54
1:C:109:ARG:HH22	1:D:24:LYS:HE3	1.73	0.54
1:C:137:ALA:N	1:C:138:PRO:CD	2.71	0.54
1:A:141:ARG:HB3	1:A:147:ARG:NH2	2.23	0.54
1:D:123:PRO:O	1:D:124:ASP:HB2	2.08	0.54
1:D:165:ARG:NH1	1:D:165:ARG:CG	2.43	0.54
1:A:43:ARG:HG3	5:A:323:HOH:O	2.08	0.53
1:C:141:ARG:HG2	5:C:420:HOH:O	2.07	0.53
1:C:32:ASP:HB3	1:C:35:VAL:HB	1.90	0.53
1:A:62:GLU:OE1	1:A:87:GLY:HA3	2.09	0.53
1:B:54:GLU:C	1:B:56:GLU:H	2.16	0.53
1:B:118:PRO:O	1:B:121:ALA:HB2	2.08	0.53
1:B:116:VAL:CA	5:B:215:HOH:O	2.57	0.53
1:A:83:VAL:O	1:A:139:LEU:HD13	2.09	0.53
1:D:33:THR:O	1:D:37:ILE:HG13	2.08	0.53
1:D:160:ARG:O	1:D:163:LEU:N	2.42	0.53
1:B:122:GLY:HA3	5:B:401:HOH:O	2.09	0.53
1:C:12:GLY:O	1:C:13:SER:C	2.50	0.53
1:C:54:GLU:HG2	1:C:54:GLU:O	2.07	0.52
1:C:160:ARG:HH11	1:C:160:ARG:CG	2.05	0.52
1:B:130:ARG:CD	5:B:369:HOH:O	2.43	0.52
1:B:10:LEU:HB3	1:B:11:PRO:HD2	1.90	0.52
1:B:62:GLU:O	1:B:66:ARG:HG2	2.10	0.52
1:C:108:VAL:CA	5:C:413:HOH:O	2.37	0.52
1:A:136:ARG:O	1:A:137:ALA:C	2.51	0.52
1:C:162:ILE:O	1:C:163:LEU:C	2.50	0.52
1:A:110:ARG:HB3	4:A:180:ADP:O4'	2.08	0.52
1:D:88:VAL:O	1:D:90:ALA:N	2.42	0.52
1:C:26:LEU:HA	5:C:219:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:VAL:HG12	1:C:108:VAL:O	2.10	0.51
1:D:44:SER:O	1:D:48:ILE:HG13	2.10	0.51
1:D:101:GLU:O	1:D:150:THR:OG1	2.28	0.51
1:B:153:ARG:HG3	5:B:437:HOH:O	2.10	0.51
1:D:152:ARG:HG3	1:D:152:ARG:HH11	1.75	0.51
1:B:63:ASP:HA	5:B:469:HOH:O	2.10	0.51
1:C:102:ILE:HG13	1:C:103:SER:N	2.26	0.51
1:B:152:ARG:HB3	5:B:249:HOH:O	2.10	0.51
1:C:44:SER:O	1:C:47:ASP:N	2.44	0.51
1:D:11:PRO:O	5:D:353:HOH:O	2.19	0.51
1:B:107:GLY:HA3	1:B:129:TYR:OH	2.11	0.50
1:D:123:PRO:HB2	1:D:128:LYS:NZ	2.26	0.50
1:A:158:VAL:O	1:A:162:ILE:HG13	2.10	0.50
1:B:38:GLU:CG	1:B:45:ILE:HG12	2.40	0.50
1:B:152:ARG:C	5:B:250:HOH:O	2.54	0.50
1:C:159:VAL:O	1:C:163:LEU:HD12	2.11	0.50
1:D:65:VAL:HG21	1:D:78:LEU:CD1	2.40	0.50
1:C:104:ALA:HA	1:C:129:TYR:CE1	2.46	0.50
1:B:153:ARG:HD2	5:B:437:HOH:O	2.10	0.50
1:C:49:PHE:CE1	1:C:54:GLU:HG3	2.46	0.50
1:B:131:ALA:O	1:B:132:LEU:C	2.54	0.50
1:D:112:GLY:O	1:D:114:ASN:N	2.45	0.50
1:B:96:THR:HG23	5:B:311:HOH:O	2.12	0.49
1:C:64:VAL:O	1:C:65:VAL:C	2.54	0.49
1:D:21:ARG:HB2	1:D:159:VAL:HG21	1.94	0.49
1:C:165:ARG:C	5:C:320:HOH:O	2.55	0.49
1:A:136:ARG:CG	1:A:136:ARG:NH1	2.65	0.49
1:A:38:GLU:HA	1:A:43:ARG:O	2.13	0.49
1:D:115:THR:O	1:D:116:VAL:HB	2.13	0.49
1:D:116:VAL:HG13	5:D:336:HOH:O	2.13	0.48
1:A:69:LEU:CD2	1:A:95:HIS:CE1	2.94	0.48
1:B:147:ARG:O	1:B:147:ARG:CG	2.54	0.48
1:A:86:PRO:HG2	1:A:87:GLY:N	2.25	0.48
1:B:10:LEU:HG	5:B:253:HOH:O	2.13	0.48
1:B:127:GLU:CG	5:B:362:HOH:O	2.49	0.48
1:D:6:VAL:HA	1:D:76:LEU:O	2.12	0.48
1:C:60:ILE:O	1:C:64:VAL:HG23	2.12	0.48
1:D:121:ALA:O	1:D:123:PRO:CD	2.59	0.48
1:C:40:ARG:NE	5:C:316:HOH:O	2.41	0.48
5:B:447:HOH:O	1:C:24:LYS:HD2	1.99	0.48
1:C:8:VAL:HB	1:C:140:TYR:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:THR:O	1:C:37:ILE:HG13	2.14	0.48
1:D:95:HIS:H	1:D:95:HIS:CD2	2.31	0.48
1:D:22:LEU:HA	1:D:159:VAL:CG1	2.44	0.48
1:B:21:ARG:HB2	1:B:159:VAL:HG21	1.95	0.48
1:B:103:SER:HB3	1:B:105:ALA:H	1.78	0.48
1:A:16:SER:N	5:A:449:HOH:O	2.47	0.47
1:B:111:THR:HG22	1:B:117:ARG:CZ	2.44	0.47
1:D:124:ASP:CG	5:D:471:HOH:O	2.57	0.47
1:A:102:ILE:HG23	1:A:102:ILE:O	2.12	0.47
1:B:46:ALA:HB2	1:B:116:VAL:HG12	1.95	0.47
1:A:50:ALA:HB1	5:C:217:HOH:O	2.14	0.47
1:A:12:GLY:HA2	4:A:180:ADP:H5'1	1.96	0.47
1:A:89:ARG:NH1	1:A:89:ARG:CG	2.74	0.47
1:D:119:LEU:CD1	5:D:283:HOH:O	2.62	0.47
5:A:332:HOH:O	1:C:128:LYS:HD3	2.13	0.47
1:A:45:ILE:HA	1:A:48:ILE:HD12	1.96	0.47
1:A:83:VAL:HG13	5:A:224:HOH:O	2.15	0.47
1:C:157:ALA:HB2	5:C:411:HOH:O	1.80	0.47
1:D:69:LEU:CD2	1:D:95:HIS:CE1	2.98	0.47
1:A:86:PRO:N	5:A:379:HOH:O	2.37	0.47
1:C:155:PRO:HG3	4:C:182:ADP:C6	2.50	0.47
1:D:82:ALA:N	5:D:465:HOH:O	2.37	0.47
1:D:125:ARG:HD3	5:D:399:HOH:O	2.15	0.47
1:A:56:GLU:CG	5:A:384:HOH:O	2.62	0.47
1:D:131:ALA:HB2	5:D:404:HOH:O	2.14	0.46
1:B:120:LEU:O	1:B:121:ALA:O	2.33	0.46
1:B:146:MET:HE2	1:B:146:MET:HB2	1.56	0.46
1:C:8:VAL:HB	1:C:140:TYR:CE1	2.51	0.46
1:C:58:ARG:HH22	1:C:81:GLY:HA3	1.80	0.46
1:D:43:ARG:NH2	1:D:52:ASP:OD1	2.45	0.46
1:A:61:GLU:CD	1:A:82:ALA:HB2	2.40	0.46
1:C:31:LEU:CD2	1:C:32:ASP:N	2.78	0.46
1:C:66:ARG:NH2	1:C:87:GLY:C	2.73	0.46
1:D:67:ALA:O	1:D:68:ALA:C	2.58	0.46
1:A:153:ARG:NH2	1:A:161:HIS:ND1	2.63	0.46
1:B:14:GLY:O	1:B:15:LYS:C	2.59	0.46
1:B:30:LEU:HA	1:B:30:LEU:HD12	1.60	0.46
1:D:11:PRO:CG	5:D:353:HOH:O	2.22	0.46
1:C:130:ARG:HH11	1:C:130:ARG:HG2	1.71	0.46
1:D:130:ARG:HH11	1:D:130:ARG:HG2	1.80	0.46
1:A:86:PRO:CG	1:A:87:GLY:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LYS:CB	5:B:370:HOH:O	2.63	0.46
1:A:109:ARG:HH11	1:A:109:ARG:HD2	1.52	0.45
1:B:54:GLU:O	1:B:56:GLU:N	2.39	0.45
1:B:117:ARG:N	1:B:118:PRO:CD	2.78	0.45
1:D:26:LEU:HB2	1:D:28:VAL:HG22	1.97	0.45
1:C:55:GLN:CB	5:C:221:HOH:O	2.58	0.45
1:D:145:THR:O	1:D:146:MET:HG2	2.16	0.45
1:B:80:GLY:O	1:B:140:TYR:OH	2.26	0.45
1:D:96:THR:HG23	1:D:146:MET:HE3	1.98	0.45
1:C:31:LEU:CD2	1:C:32:ASP:H	2.27	0.45
1:A:141:ARG:HD2	1:A:147:ARG:NH2	2.13	0.45
1:A:141:ARG:CG	1:A:147:ARG:NH2	2.79	0.45
1:B:55:GLN:CD	1:B:55:GLN:H	2.25	0.45
1:B:103:SER:HB2	1:B:106:GLU:H	1.82	0.45
1:C:78:LEU:HD21	1:C:82:ALA:HB3	1.97	0.45
1:B:103:SER:CB	1:B:105:ALA:H	2.29	0.45
1:C:24:LYS:C	1:C:26:LEU:H	2.25	0.45
1:C:86:PRO:HG3	1:C:89:ARG:NH2	2.32	0.45
1:C:52:ASP:HB3	5:C:274:HOH:O	2.17	0.45
1:A:108:VAL:O	1:A:108:VAL:CG1	2.65	0.45
1:B:25:ALA:HB1	1:B:163:LEU:HD11	2.00	0.45
1:B:46:ALA:H	1:B:116:VAL:HG12	1.82	0.45
1:B:121:ALA:CB	1:D:123:PRO:HG3	2.46	0.45
1:C:47:ASP:O	1:C:48:ILE:CG1	2.63	0.45
1:D:72:HIS:NE2	1:D:74:GLY:CA	2.79	0.45
1:C:106:GLU:O	1:C:110:ARG:HG3	2.17	0.44
1:C:141:ARG:HD3	5:C:420:HOH:O	2.17	0.44
1:A:128:LYS:HG2	1:C:43:ARG:NH1	2.32	0.44
1:B:6:VAL:HG13	1:B:76:LEU:HD23	1.98	0.44
1:B:20:ARG:HA	1:B:30:LEU:HD22	1.99	0.44
1:A:102:ILE:O	1:A:102:ILE:CG2	2.63	0.44
1:D:69:LEU:HD22	1:D:95:HIS:CE1	2.51	0.44
1:D:102:ILE:HD11	1:D:106:GLU:CG	2.47	0.44
1:D:113:GLY:C	5:D:328:HOH:O	2.60	0.44
1:D:124:ASP:OD1	1:D:124:ASP:C	2.58	0.44
1:C:14:GLY:HA2	4:C:182:ADP:O2A	2.16	0.44
1:A:20:ARG:CD	5:B:293:HOH:O	2.51	0.44
1:A:49:PHE:HE1	1:A:54:GLU:HG2	1.83	0.44
1:C:15:LYS:CG	4:C:182:ADP:O1B	2.61	0.44
1:C:166:LEU:C	5:C:321:HOH:O	2.61	0.44
1:B:6:VAL:HA	1:B:76:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:PRO:HB2	1:D:128:LYS:HZ3	1.82	0.44
1:A:19:GLY:C	1:A:30:LEU:HD22	2.42	0.44
1:A:26:LEU:HA	1:A:26:LEU:HD23	1.58	0.44
1:C:48:ILE:HG22	1:C:57:PHE:HB2	1.99	0.43
1:A:148:VAL:HG11	1:A:158:VAL:HG13	2.00	0.43
1:B:7:LEU:HD23	1:B:98:VAL:HB	2.00	0.43
1:B:53:GLY:HA3	5:D:471:HOH:O	2.19	0.43
1:C:157:ALA:O	1:C:158:VAL:C	2.60	0.43
1:D:114:ASN:OD1	5:D:232:HOH:O	2.21	0.43
1:D:115:THR:O	1:D:116:VAL:CB	2.66	0.43
1:B:116:VAL:HA	5:B:215:HOH:O	2.18	0.43
1:C:58:ARG:HH11	1:C:58:ARG:CG	2.32	0.43
1:C:131:ALA:O	1:C:134:ALA:N	2.51	0.43
1:B:105:ALA:O	1:B:109:ARG:HG3	2.18	0.43
1:A:57:PHE:CD2	1:A:58:ARG:HD3	2.52	0.43
1:A:61:GLU:O	1:A:62:GLU:C	2.62	0.43
1:B:149:ASP:OD1	1:B:151:ASN:ND2	2.33	0.43
1:D:65:VAL:O	1:D:66:ARG:C	2.60	0.43
1:B:111:THR:HB	1:B:117:ARG:HD3	2.01	0.43
1:C:140:TYR:C	1:C:142:ARG:H	2.26	0.43
1:A:108:VAL:O	1:A:108:VAL:HG12	2.16	0.43
1:B:166:LEU:C	5:B:451:HOH:O	2.62	0.43
1:D:45:ILE:HD13	1:D:57:PHE:HE1	1.83	0.43
1:D:120:LEU:O	1:D:122:GLY:N	2.52	0.43
1:C:15:LYS:O	1:C:19:GLY:HA3	2.19	0.43
1:A:21:ARG:HH22	1:B:106:GLU:CD	2.26	0.42
1:A:106:GLU:O	1:A:109:ARG:N	2.52	0.42
1:B:111:THR:OG1	1:B:125:ARG:NH1	2.52	0.42
1:C:41:THR:O	1:C:43:ARG:N	2.52	0.42
1:B:23:ALA:HB1	1:B:28:VAL:O	2.18	0.42
1:D:130:ARG:HG2	1:D:130:ARG:NH1	2.33	0.42
1:B:135:LYS:HB3	5:B:370:HOH:O	2.18	0.42
1:C:160:ARG:NH1	5:C:345:HOH:O	2.52	0.42
1:A:56:GLU:CD	5:A:384:HOH:O	2.62	0.42
1:A:56:GLU:HG3	1:A:60:ILE:HD11	2.01	0.42
1:B:22:LEU:HD23	1:B:75:VAL:HG21	2.01	0.42
1:D:122:GLY:O	1:D:123:PRO:C	2.61	0.42
1:A:112:GLY:HA3	1:B:20:ARG:NE	2.34	0.42
1:B:85:SER:HA	1:B:86:PRO:HD2	1.75	0.42
1:D:61:GLU:CD	1:D:82:ALA:HB2	2.44	0.42
1:A:37:ILE:O	1:A:41:THR:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLN:CD	1:A:55:GLN:N	2.72	0.42
1:C:85:SER:HA	1:C:86:PRO:HD3	1.95	0.42
1:C:127:GLU:CA	1:C:130:ARG:HB2	2.49	0.42
1:A:107:GLY:HA3	1:A:129:TYR:OH	2.19	0.42
1:B:116:VAL:O	1:B:117:ARG:HB2	2.20	0.42
1:C:20:ARG:O	1:C:23:ALA:HB3	2.19	0.42
1:C:152:ARG:O	1:C:153:ARG:C	2.61	0.42
1:D:162:ILE:O	1:D:166:LEU:HG	2.20	0.42
1:A:132:LEU:HA	1:A:132:LEU:HD12	1.16	0.41
1:D:137:ALA:O	1:D:141:ARG:HG3	2.20	0.41
1:A:125:ARG:HH11	1:A:125:ARG:HD2	1.55	0.41
1:B:2:ALA:HA	1:B:3:PRO:HD3	1.86	0.41
1:C:159:VAL:HG12	1:C:163:LEU:HD12	2.02	0.41
1:D:129:TYR:O	1:D:130:ARG:C	2.57	0.41
1:D:160:ARG:O	1:D:161:HIS:C	2.63	0.41
1:A:154:ASN:O	1:A:155:PRO:C	2.61	0.41
1:B:18:ILE:O	1:B:22:LEU:CB	2.69	0.41
1:B:85:SER:O	1:B:86:PRO:C	2.63	0.41
1:D:130:ARG:HH11	1:D:130:ARG:CG	2.34	0.41
1:B:13:SER:HB2	1:B:100:LEU:HB3	2.01	0.41
1:C:22:LEU:O	1:C:26:LEU:HB2	2.20	0.41
1:D:122:GLY:O	1:D:124:ASP:N	2.53	0.41
1:A:101:GLU:HG3	1:A:148:VAL:O	2.21	0.41
1:D:59:ARG:HE	1:D:59:ARG:HB3	1.76	0.41
1:D:119:LEU:HD12	5:D:283:HOH:O	2.19	0.41
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.52	0.41
1:B:54:GLU:C	1:B:56:GLU:N	2.79	0.41
1:B:122:GLY:HA3	1:B:123:PRO:HD3	1.93	0.41
1:A:46:ALA:O	1:A:47:ASP:C	2.64	0.41
1:A:99:TYR:CE1	1:A:140:TYR:HB3	2.56	0.41
1:C:66:ARG:HH22	1:C:87:GLY:C	2.28	0.41
1:B:125:ARG:O	1:B:126:ALA:C	2.63	0.41
1:D:11:PRO:HB3	5:D:242:HOH:O	2.21	0.41
1:C:18:ILE:O	1:C:22:LEU:HB3	2.21	0.41
1:C:92:LEU:HA	1:C:92:LEU:HD23	1.51	0.41
4:C:182:ADP:O2'	4:D:183:ADP:H1'	2.21	0.41
1:A:57:PHE:HD2	1:A:58:ARG:HD3	1.85	0.41
1:B:34:ASP:O	1:B:45:ILE:HD11	2.20	0.41
1:C:69:LEU:HA	1:C:69:LEU:HD23	1.89	0.41
1:B:136:ARG:HH11	1:B:136:ARG:HD3	1.73	0.40
1:C:65:VAL:O	1:C:66:ARG:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:VAL:C	1:D:90:ALA:N	2.78	0.40
1:B:147:ARG:HH11	1:B:147:ARG:HD2	1.67	0.40
1:D:123:PRO:O	1:D:124:ASP:CB	2.70	0.40
1:A:22:LEU:O	1:A:26:LEU:HG	2.21	0.40
1:A:56:GLU:HG3	1:A:60:ILE:CD1	2.51	0.40
1:A:126:ALA:O	1:A:130:ARG:HG3	2.21	0.40
1:B:62:GLU:HG3	1:B:88:VAL:CG2	2.52	0.40
1:B:149:ASP:HB3	1:B:153:ARG:HH12	1.86	0.40
1:C:58:ARG:NH2	1:C:81:GLY:HA3	2.37	0.40
1:C:79:GLY:C	5:C:331:HOH:O	2.63	0.40
1:C:146:MET:CE	1:C:165:ARG:HB3	2.52	0.40
1:D:10:LEU:HB3	5:D:353:HOH:O	2.22	0.40

All (4) 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)
5:A:436:HOH:O	5:B:441:HOH:O[4_456]	1.71	0.49
1:B:135:LYS:CD	5:A:436:HOH:O[4_556]	1.93	0.27
1:C:96:THR:OG1	1:D:130:ARG:NH2[3_655]	2.04	0.16
5:C:287:HOH:O	5:D:286:HOH:O[3_555]	2.07	0.13

## 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	152/176 (86%)	132 (87%)	14 (9%)	6 (4%)	<b>2</b> <b>8</b>
1	B	163/176 (93%)	133 (82%)	17 (10%)	13 (8%)	<b>1</b> <b>1</b>
1	C	151/176 (86%)	129 (85%)	14 (9%)	8 (5%)	<b>1</b> <b>5</b>
1	D	163/176 (93%)	136 (83%)	12 (7%)	15 (9%)	<b>0</b> <b>1</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	629/704 (89%)	530 (84%)	57 (9%)	42 (7%)	<b>1</b> <b>3</b>

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	B	46	ALA
1	B	115	THR
1	B	121	ALA
1	B	132	LEU
1	B	151	ASN
1	C	48	ILE
1	C	80	GLY
1	C	81	GLY
1	C	107	GLY
1	D	74	GLY
1	D	114	ASN
1	D	115	THR
1	A	50	ALA
1	A	54	GLU
1	A	112	GLY
1	B	55	GLN
1	B	113	GLY
1	B	116	VAL
1	C	51	THR
1	D	27	GLY
1	D	80	GLY
1	D	116	VAL
1	D	123	PRO
1	A	41	THR
1	A	49	PHE
1	B	87	GLY
1	B	114	ASN
1	B	122	GLY
1	D	69	LEU
1	D	103	SER
1	C	153	ARG
1	D	89	ARG
1	D	122	GLY
1	B	18	ILE
1	D	121	ALA
1	D	124	ASP

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Mol	Chain	Res	Type
1	C	45	ILE
1	D	113	GLY
1	D	117	ARG
1	B	86	PRO
1	C	155	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
1	A	116/132 (88%)	93 (80%)	23 (20%)	<b>1</b> <b>5</b>
1	B	123/132 (93%)	106 (86%)	17 (14%)	<b>3</b> <b>12</b>
1	C	115/132 (87%)	91 (79%)	24 (21%)	<b>1</b> <b>4</b>
1	D	122/132 (92%)	102 (84%)	20 (16%)	<b>2</b> <b>8</b>
All	All	476/528 (90%)	392 (82%)	84 (18%)	<b>2</b> <b>7</b>

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	24	LYS
1	A	39	GLN
1	A	40	ARG
1	A	44	SER
1	A	45	ILE
1	A	51	THR
1	A	52	ASP
1	A	54	GLU
1	A	55	GLN
1	A	59	ARG
1	A	63	ASP
1	A	78	LEU
1	A	89	ARG
1	A	101	GLU
1	A	102	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	109	ARG
1	A	130	ARG
1	A	135	LYS
1	A	136	ARG
1	A	154	ASN
1	A	165	ARG
1	A	166	LEU
1	B	20	ARG
1	B	21	ARG
1	B	37	ILE
1	B	40	ARG
1	B	55	GLN
1	B	59	ARG
1	B	92	LEU
1	B	96	THR
1	B	114	ASN
1	B	115	THR
1	B	132	LEU
1	B	136	ARG
1	B	141	ARG
1	B	142	ARG
1	B	147	ARG
1	B	153	ARG
1	B	165	ARG
1	C	4	LYS
1	C	15	LYS
1	C	20	ARG
1	C	26	LEU
1	C	31	LEU
1	C	38	GLU
1	C	39	GLN
1	C	43	ARG
1	C	45	ILE
1	C	55	GLN
1	C	57	PHE
1	C	58	ARG
1	C	59	ARG
1	C	60	ILE
1	C	63	ASP
1	C	84	THR
1	C	102	ILE
1	C	125	ARG

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Mol	Chain	Res	Type
1	C	130	ARG
1	C	132	LEU
1	C	136	ARG
1	C	142	ARG
1	C	160	ARG
1	C	166	LEU
1	D	4	LYS
1	D	15	LYS
1	D	16	SER
1	D	21	ARG
1	D	22	LEU
1	D	39	GLN
1	D	45	ILE
1	D	47	ASP
1	D	52	ASP
1	D	55	GLN
1	D	60	ILE
1	D	64	VAL
1	D	66	ARG
1	D	71	ASP
1	D	102	ILE
1	D	127	GLU
1	D	130	ARG
1	D	152	ARG
1	D	153	ARG
1	D	165	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	B	39	GLN
1	C	151	ASN
1	C	161	HIS
1	D	39	GLN
1	D	55	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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
4	ADP	C	182	2	28,29,29	1.35	4 (14%)	43,45,45	2.81	20 (46%)
4	ADP	B	181	2	28,29,29	1.35	3 (10%)	43,45,45	3.04	20 (46%)
4	ADP	A	180	2	28,29,29	1.37	3 (10%)	43,45,45	2.99	22 (51%)
4	ADP	D	183	2	28,29,29	1.14	2 (7%)	43,45,45	2.40	9 (20%)

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
4	ADP	C	182	2	-	2/16/32/32	0/3/3/3
4	ADP	B	181	2	-	3/16/32/32	0/3/3/3
4	ADP	A	180	2	-	4/16/32/32	0/3/3/3
4	ADP	D	183	2	-	4/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	181	ADP	C8-N7	3.85	1.39	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	180	ADP	C5-N7	-3.75	1.32	1.39
4	C	182	ADP	PA-O3A	3.62	1.63	1.59
4	A	180	ADP	C8-N9	-3.34	1.31	1.37
4	B	181	ADP	C8-N9	-3.24	1.32	1.37
4	D	183	ADP	PA-O3A	3.06	1.62	1.59
4	D	183	ADP	C8-N7	2.98	1.37	1.31
4	A	180	ADP	C8-N7	2.43	1.36	1.31
4	C	182	ADP	C8-N7	2.28	1.36	1.31
4	C	182	ADP	C8-N9	-2.21	1.33	1.37
4	C	182	ADP	PB-O3B	-2.10	1.47	1.54
4	B	181	ADP	C4-N9	-2.01	1.33	1.37

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	181	ADP	C4-C5-N7	-8.55	100.81	110.58
4	B	181	ADP	C5-C4-N3	-7.95	115.77	126.72
4	A	180	ADP	C5-C4-N3	-7.62	116.23	126.72
4	D	183	ADP	N3-C2-N1	-7.25	117.60	128.58
4	D	183	ADP	C5-C4-N3	-7.20	116.80	126.72
4	B	181	ADP	C5-C4-N9	6.81	113.24	105.81
4	C	182	ADP	N9-C8-N7	-6.25	105.07	113.94
4	C	182	ADP	C4-N9-C8	6.25	112.30	105.74
4	C	182	ADP	N3-C2-N1	-5.99	119.51	128.58
4	A	180	ADP	N9-C8-N7	-5.91	105.55	113.94
4	A	180	ADP	C5-N7-C8	5.87	112.67	103.45
4	C	182	ADP	C2'-C3'-C4'	5.63	113.48	102.61
4	D	183	ADP	C2-N3-C4	5.45	125.13	111.83
4	A	180	ADP	C4-C5-N7	-5.38	104.44	110.58
4	C	182	ADP	O3A-PA-O1A	-5.33	94.66	110.70
4	A	180	ADP	N3-C4-N9	4.82	135.36	127.17
4	D	183	ADP	C5-C4-N9	4.61	110.83	105.81
4	B	181	ADP	C5-N7-C8	4.60	110.69	103.45
4	A	180	ADP	O4'-C4'-C3'	-4.55	96.12	105.15
4	B	181	ADP	O3A-PA-O1A	-4.52	97.09	110.70
4	C	182	ADP	O2A-PA-O1A	4.37	132.77	112.44
4	C	182	ADP	C5-N7-C8	4.34	110.27	103.45
4	B	181	ADP	O2'-C2'-C3'	-4.08	98.72	111.82
4	A	180	ADP	O4'-C4'-C5'	-3.99	96.54	109.33
4	B	181	ADP	N9-C8-N7	-3.96	108.32	113.94
4	B	181	ADP	C2-N3-C4	3.89	121.32	111.83
4	A	180	ADP	N3-C2-N1	-3.87	122.73	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	180	ADP	C2-N3-C4	3.83	121.19	111.83
4	C	182	ADP	C2-N1-C6	3.83	125.02	118.73
4	D	183	ADP	O2'-C2'-C3'	-3.71	99.93	111.82
4	D	183	ADP	C4-C5-N7	-3.70	106.35	110.58
4	C	182	ADP	C4-C5-N7	-3.69	106.36	110.58
4	A	180	ADP	C2'-C3'-C4'	3.61	109.58	102.61
4	B	181	ADP	O2A-PA-O3A	3.56	116.90	107.27
4	B	181	ADP	N6-C6-N1	-3.53	110.52	118.38
4	C	182	ADP	C3'-C2'-C1'	-3.43	94.98	101.46
4	A	180	ADP	O4'-C1'-C2'	-3.41	99.33	106.62
4	A	180	ADP	O2B-PB-O1B	3.40	124.07	110.83
4	B	181	ADP	C6-C5-N7	3.36	138.56	132.09
4	C	182	ADP	C4-N9-C1'	-3.34	118.82	126.63
4	A	180	ADP	O3'-C3'-C2'	-3.31	101.20	111.82
4	A	180	ADP	C4-N9-C8	3.17	109.07	105.74
4	C	182	ADP	O4'-C4'-C3'	-3.10	99.00	105.15
4	B	181	ADP	O3'-C3'-C2'	-3.10	101.88	111.82
4	A	180	ADP	O4'-C1'-N9	-3.07	102.19	108.09
4	B	181	ADP	O5'-C5'-C4'	-2.95	98.94	108.99
4	B	181	ADP	O3A-PB-O1B	-2.91	95.74	111.04
4	D	183	ADP	O3'-C3'-C4'	-2.88	102.82	111.08
4	A	180	ADP	O3A-PA-O1A	-2.86	102.10	110.70
4	A	180	ADP	C4'-O4'-C1'	2.82	115.69	109.47
4	C	182	ADP	C2-N3-C4	2.75	118.54	111.83
4	D	183	ADP	N3-C4-N9	2.74	131.84	127.17
4	B	181	ADP	O2A-PA-O1A	2.60	124.54	112.44
4	A	180	ADP	O5'-C5'-C4'	-2.57	100.23	108.99
4	C	182	ADP	PA-O5'-C5'	2.56	136.01	121.35
4	B	181	ADP	C5-C6-N6	2.54	129.57	123.29
4	B	181	ADP	C6-C5-C4	2.53	120.63	117.18
4	C	182	ADP	C5-C4-N3	-2.51	123.26	126.72
4	B	181	ADP	O3B-PB-O3A	2.47	112.94	104.64
4	C	182	ADP	O3B-PB-O3A	-2.45	96.43	104.64
4	A	180	ADP	O3B-PB-O1B	-2.38	101.56	110.83
4	A	180	ADP	C6-C5-C4	2.35	120.39	117.18
4	A	180	ADP	O2A-PA-O1A	2.31	123.20	112.44
4	B	181	ADP	O4'-C1'-N9	-2.24	103.78	108.09
4	B	181	ADP	N3-C4-N9	2.24	130.97	127.17
4	C	182	ADP	N3-C4-N9	2.20	130.91	127.17
4	C	182	ADP	O2B-PB-O3A	2.16	111.89	104.64
4	C	182	ADP	O2B-PB-O1B	2.14	119.17	110.83
4	A	180	ADP	C5-C4-N9	2.14	108.14	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	183	ADP	C2-N1-C6	2.05	122.09	118.73
4	C	182	ADP	C6-C5-N7	2.02	135.99	132.09

There are no chirality outliers.

All (13) torsion outliers are listed below:

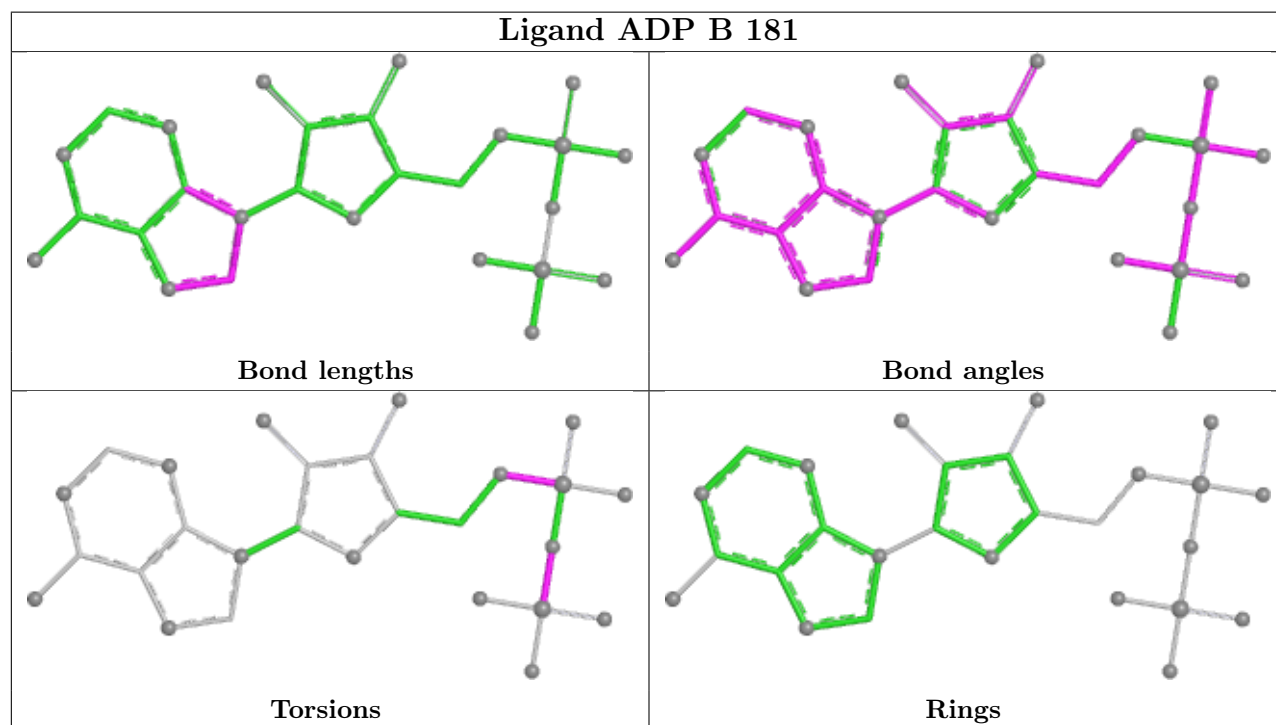
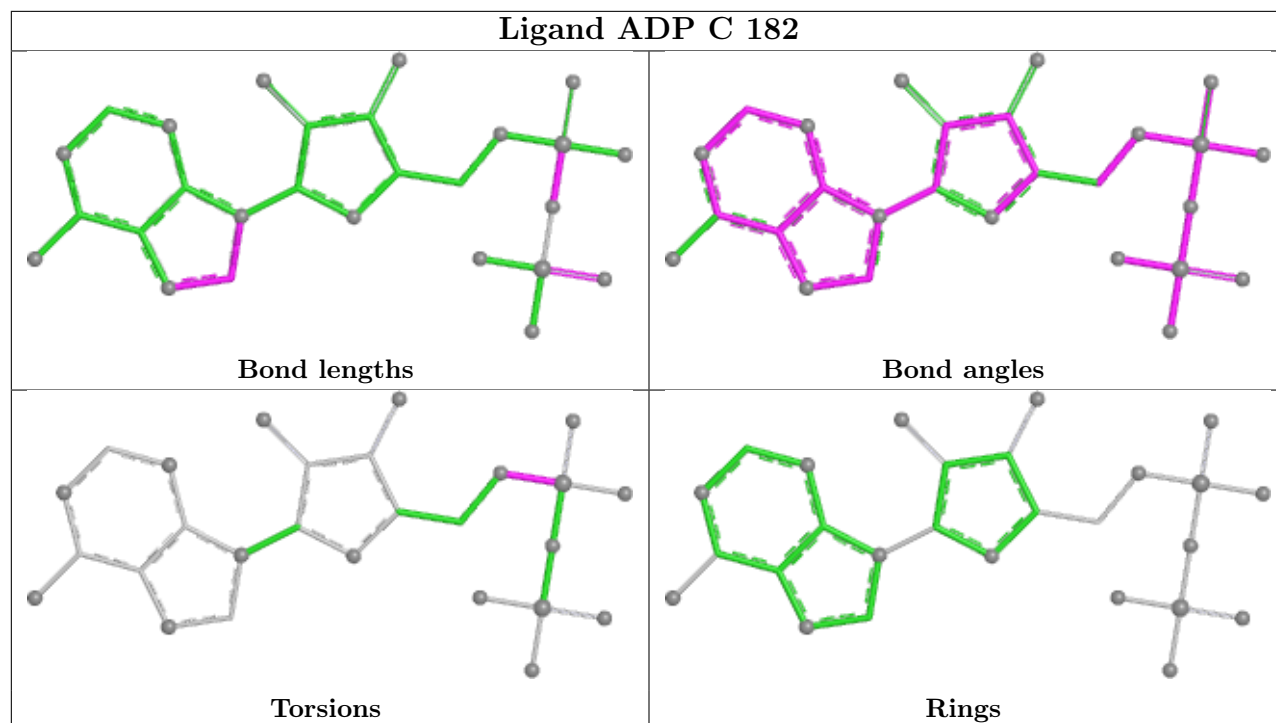
Mol	Chain	Res	Type	Atoms
4	A	180	ADP	C5'-O5'-PA-O1A
4	B	181	ADP	C5'-O5'-PA-O1A
4	C	182	ADP	C5'-O5'-PA-O1A
4	D	183	ADP	PA-O3A-PB-O2B
4	D	183	ADP	C5'-O5'-PA-O1A
4	B	181	ADP	PA-O3A-PB-O1B
4	B	181	ADP	PA-O3A-PB-O2B
4	A	180	ADP	C5'-O5'-PA-O3A
4	C	182	ADP	C5'-O5'-PA-O3A
4	D	183	ADP	C5'-O5'-PA-O2A
4	A	180	ADP	PA-O3A-PB-O1B
4	A	180	ADP	PA-O3A-PB-O3B
4	D	183	ADP	PA-O3A-PB-O1B

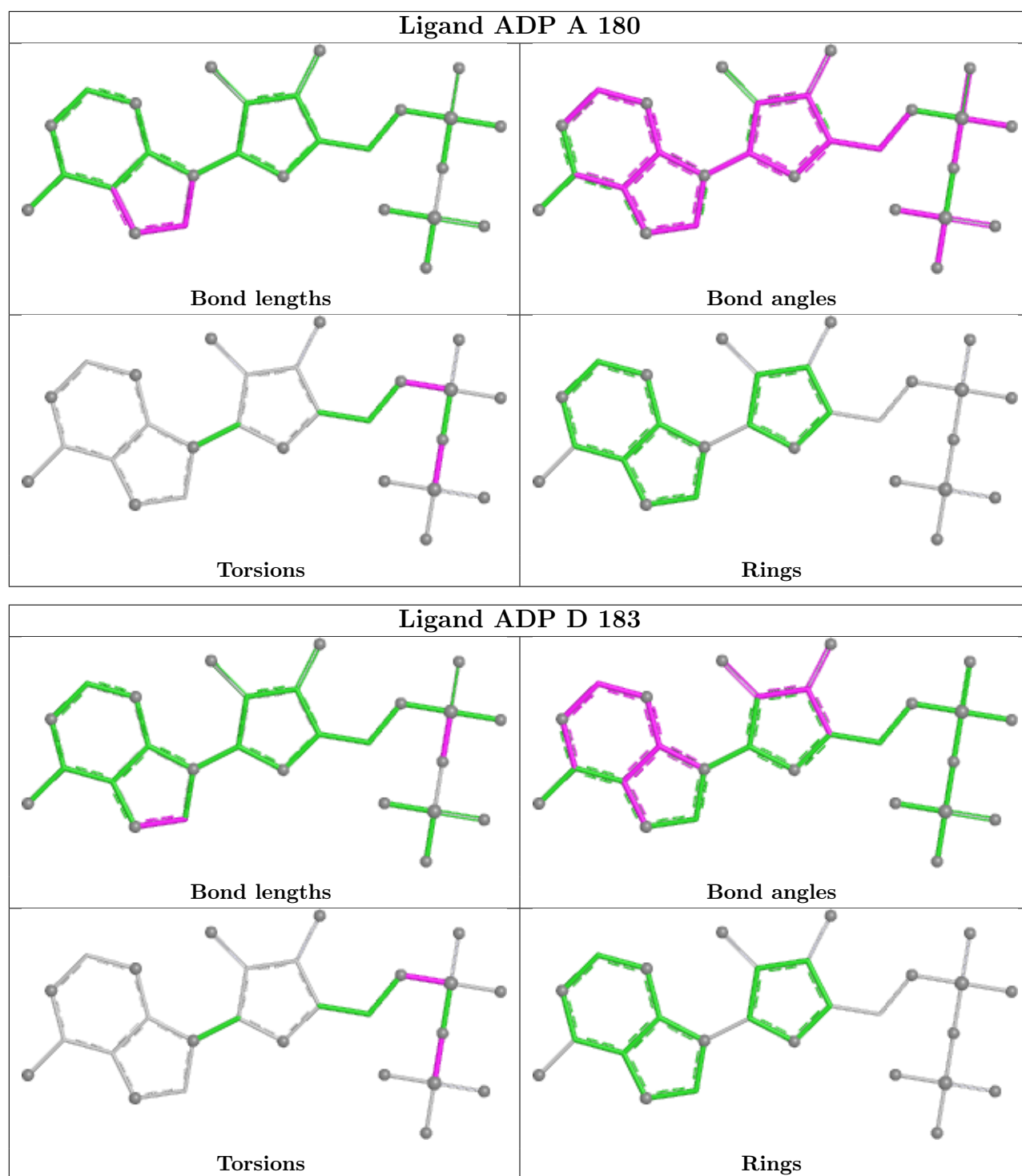
There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	182	ADP	8	0
4	B	181	ADP	2	0
4	A	180	ADP	6	0
4	D	183	ADP	6	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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	156/176 (88%)	-0.67	0 <a href="#">100</a> <a href="#">100</a>	12, 32, 53, 68	0
1	B	165/176 (93%)	-0.72	0 <a href="#">100</a> <a href="#">100</a>	9, 28, 46, 62	0
1	C	155/176 (88%)	-0.53	1 (0%) <a href="#">85</a> <a href="#">80</a>	18, 34, 61, 83	0
1	D	165/176 (93%)	-0.44	2 (1%) <a href="#">76</a> <a href="#">68</a>	20, 36, 54, 68	0
All	All	641/704 (91%)	-0.59	3 (0%) <a href="#">87</a> <a href="#">82</a>	9, 33, 53, 83	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	GLY	3.1
1	D	122	GLY	2.7
1	D	115	THR	2.3

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

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

### 6.3 Carbohydrates [i](#)

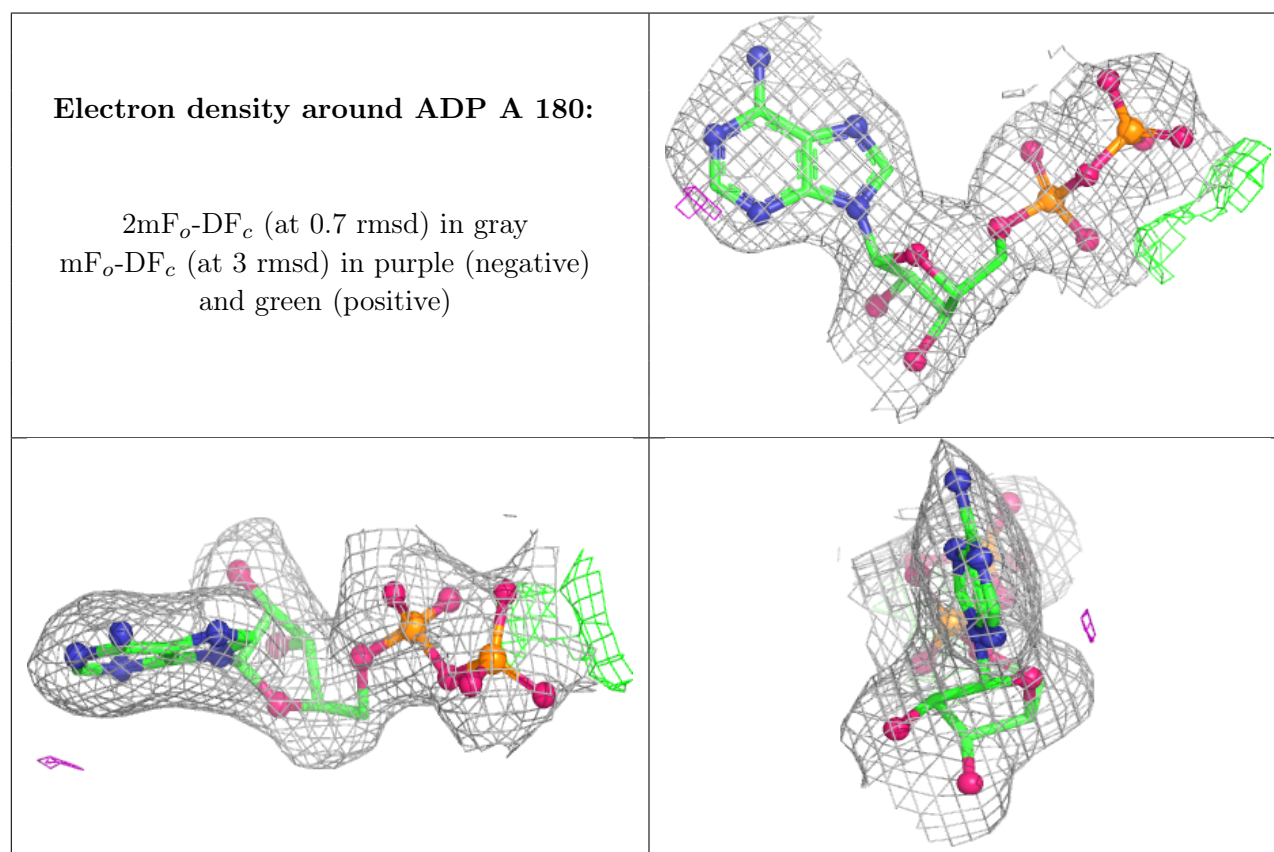
There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

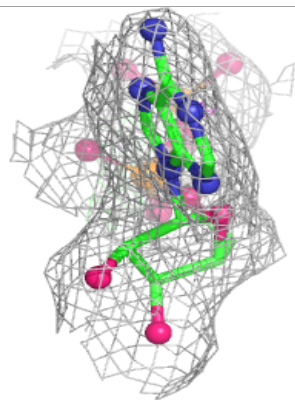
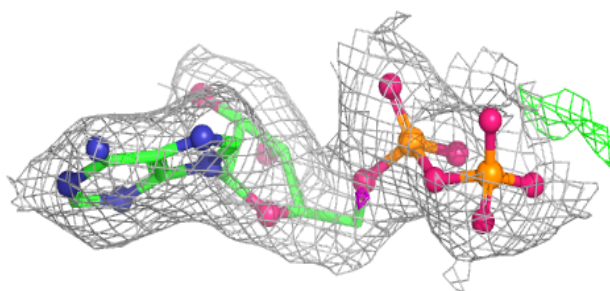
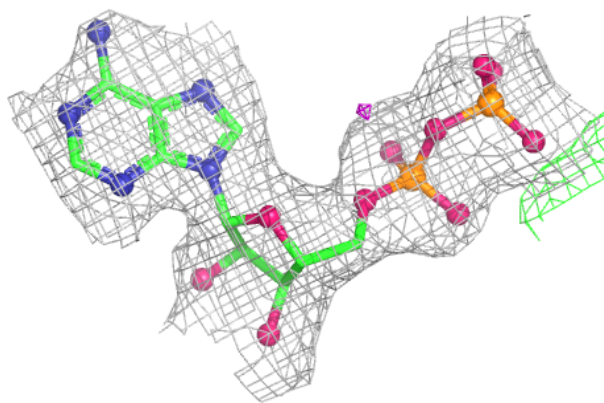
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	190	1/1	0.83	0.17	22,22,22,22	0
2	MG	C	202	1/1	0.87	0.19	29,29,29,29	0
2	MG	D	208	1/1	0.87	0.20	41,41,41,41	0
3	CL	A	193	1/1	0.91	0.07	46,46,46,46	0
2	MG	B	196	1/1	0.94	0.12	15,15,15,15	0
3	CL	B	199	1/1	0.96	0.05	26,26,26,26	0
3	CL	D	211	1/1	0.96	0.08	34,34,34,34	0
4	ADP	A	180	27/27	0.98	0.05	10,16,25,32	0
4	ADP	C	182	27/27	0.98	0.05	7,29,43,54	0
4	ADP	D	183	27/27	0.98	0.05	17,33,49,52	0
4	ADP	B	181	27/27	0.99	0.05	10,23,32,36	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.

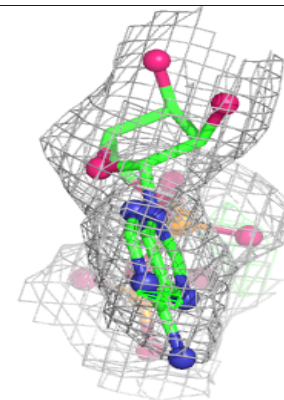
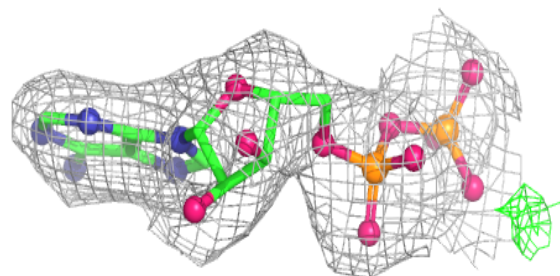
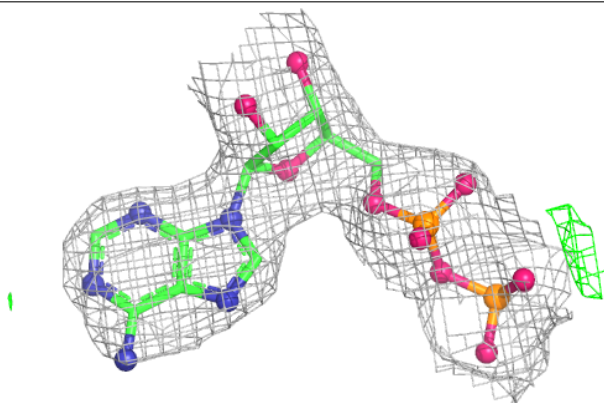


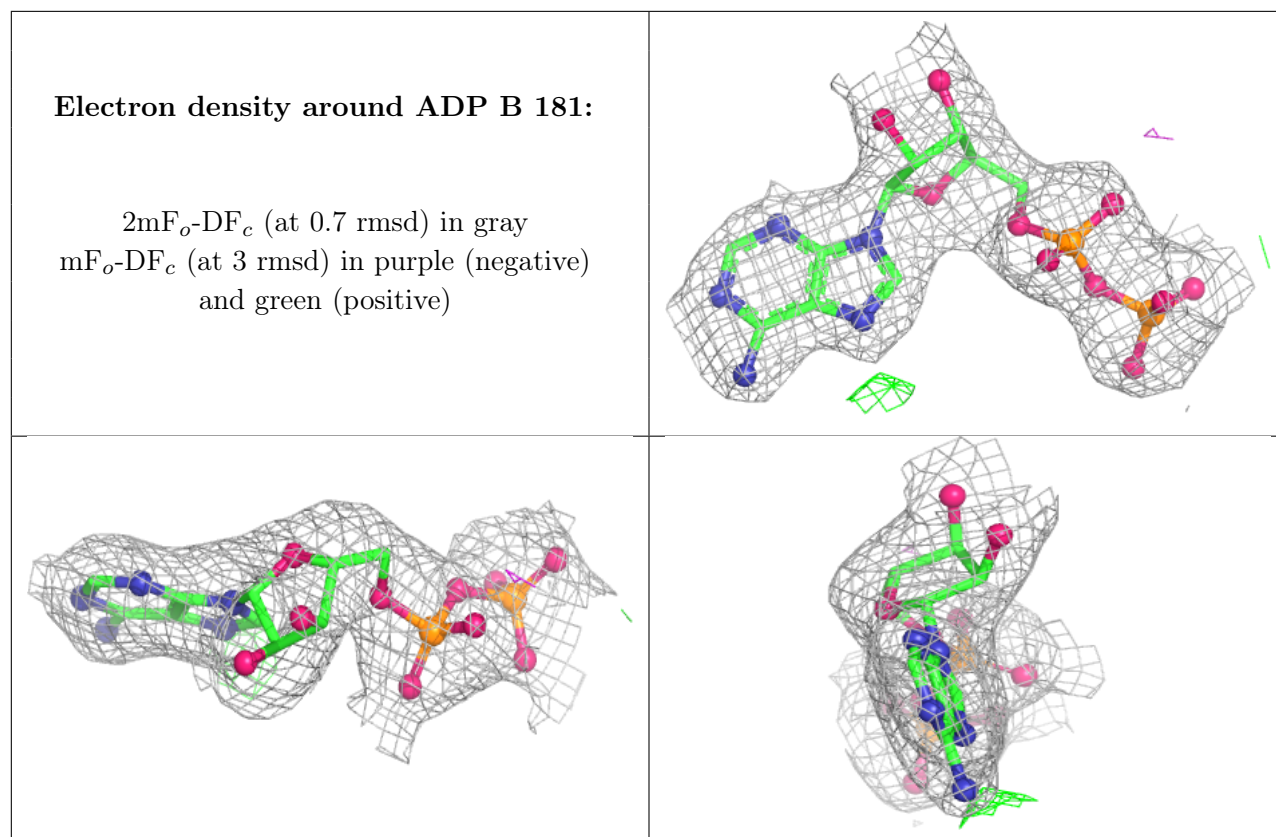
**Electron density around ADP C 182:**

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

**Electron density around ADP D 183:**

$2mF_o-DF_c$  (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.