WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 12:30 PM EDT

PDB ID	:	2DFT
Title	:	Structure of shikimate kinase from Mycobacterium tuberculosis complexed with ADP and Mg at 2.8 angstrons 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)

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

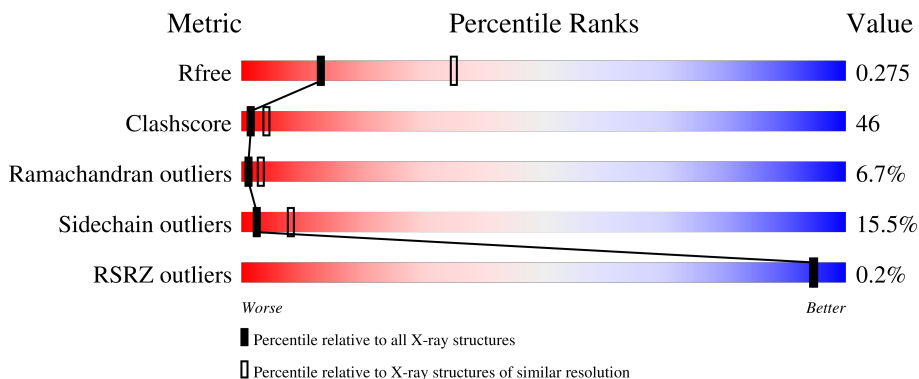|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance   ⓘ

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

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Rfree		0.275
Clashscore		46
Ramachandran outliers		6.7%
Sidechain outliers		15.5%
RSRZ outliers		0.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 >=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	A	176	33% 36% 16% • 11%
1	B	176	35% 37% 16% 6% 6%
1	C	176	24% 41% 16% 6% 12%
1	D	176	% 32% 39% 16% 7% 6%

2 Entry composition ⓘ

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

- Molecule 2 is MAGNESIUM ION (three-letter code: 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 (three-letter code: 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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

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

- Molecule 5 is water.

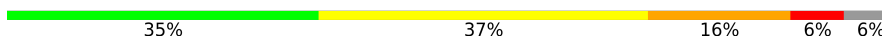| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total 60	O 60	0	0
5	B	85	Total 85	O 85	0	0
5	C	51	Total 51	O 51	0	0
5	D	64	Total 64	O 64	0	0

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:
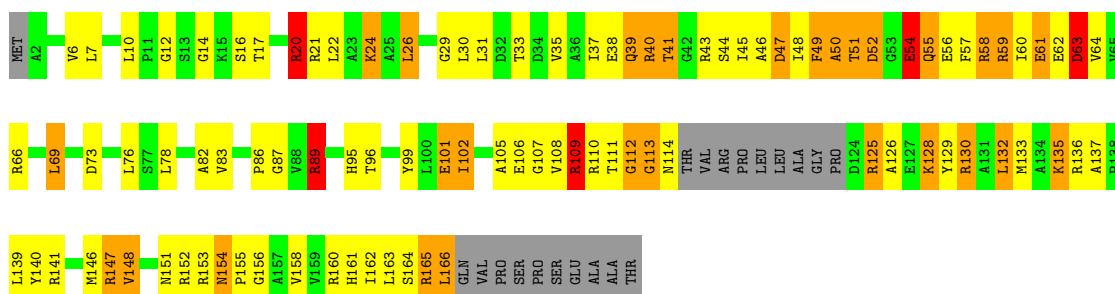
- Molecule 1: Shikimate kinase

Chain B:
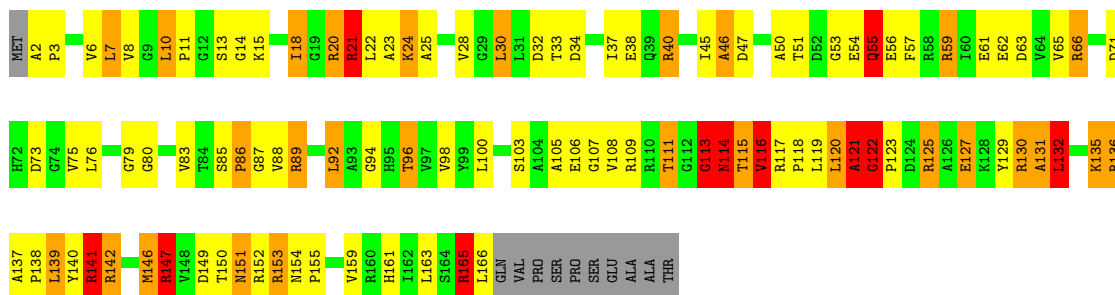
- Molecule 1: Shikimate kinase

Chain C:

• Molecule 1: Shikimate kinase

%

Chain D:

32% 39% 16% 7% 6%

MET A2 P3 K4 A5 V6 L10 P11 G12 S13 G14 K15 S16 T17 R20 R21 L22 A23 K24 A25 L26 G27 V28 L31 D32 T33 D34 V35 A36 I37 E38 Q39 R40 R43 S44 I45 A46 D47 I48 D52 G53 E54 Q55 E56 F57 R58 R59 I60 V65 R66 A67 A68 L69 A70

D71 H72 D73 G74 V75 L76 S77 L78 G79 G80 G81 A82 V88 R89 A90 G94 H95 V98 Y99 L100 E101 I102 S103 E106 G107 V108 R109 R110 T111 G112 G113 N114 T115 V116 R117 P118 L119 L120 A121 G122 P123 D124 R125 A126 E127 K128 Y129 R130 A131 L132 M133 A134 K135 R136 A137 P138

R141 R142 V143 A144 T145 M146 R147 T150 N151 R152 R153 N154 P155 V159 R160 H161 I162 L163 S164 R165 L166 GLN VAL PRO SER PRO SER GLU ALA ALA THR

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.62Å 62.20Å 170.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.17 – 2.80 57.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (57.17-2.80) 99.7 (57.12-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.81Å)	Xtriage
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 (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5152	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage'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.*

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[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: CL, ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	1.37	2/1176 (0.2%)	2.04	38/1584 (2.4%)
1	B	1.33	5/1243 (0.4%)	1.92	33/1679 (2.0%)
1	C	1.44	7/1168 (0.6%)	2.03	35/1573 (2.2%)
1	D	1.39	6/1240 (0.5%)	2.01	43/1674 (2.6%)
All	All	1.38	20/4827 (0.4%)	2.00	149/6510 (2.3%)

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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2	ALA	CA-CB	7.69	1.68	1.52
1	B	83	VAL	CB-CG1	-6.63	1.39	1.52
1	B	127	GLU	CG-CD	6.31	1.61	1.51
1	D	116	VAL	CB-CG2	6.00	1.65	1.52
1	D	129	TYR	CB-CG	-5.91	1.42	1.51
1	C	59	ARG	CB-CG	5.74	1.68	1.52
1	D	54	GLU	CB-CG	-5.72	1.41	1.52
1	C	84	THR	CB-CG2	5.63	1.71	1.52
1	A	6	VAL	CB-CG2	5.54	1.64	1.52
1	B	8	VAL	CB-CG2	5.49	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	59	ARG	CG-CD	5.43	1.65	1.51
1	B	135	LYS	CB-CG	5.25	1.66	1.52
1	C	62	GLU	CD-OE2	5.25	1.31	1.25
1	C	106	GLU	CD-OE2	5.24	1.31	1.25
1	C	130	ARG	CG-CD	5.20	1.65	1.51
1	B	130	ARG	CG-CD	5.13	1.64	1.51
1	D	55	GLN	CG-CD	5.13	1.62	1.51
1	D	99	TYR	CD2-CE2	5.02	1.46	1.39
1	A	135	LYS	CD-CE	5.01	1.63	1.51
1	C	91	ALA	CA-CB	-5.00	1.42	1.52

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	NE-CZ-NH1	-15.45	112.58	120.30
1	C	20	ARG	NE-CZ-NH2	-13.97	113.31	120.30
1	A	20	ARG	NE-CZ-NH2	-13.57	113.52	120.30
1	D	21	ARG	NE-CZ-NH2	-12.74	113.93	120.30
1	D	130	ARG	NE-CZ-NH1	12.73	126.66	120.30
1	B	21	ARG	NE-CZ-NH1	-12.48	114.06	120.30
1	C	43	ARG	NE-CZ-NH2	-12.19	114.21	120.30
1	C	66	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	D	152	ARG	NE-CZ-NH1	11.73	126.16	120.30
1	C	20	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	B	47	ASP	CB-CG-OD2	-11.52	107.93	118.30
1	A	89	ARG	NE-CZ-NH1	11.24	125.92	120.30
1	C	160	ARG	NE-CZ-NH1	-10.96	114.82	120.30
1	B	66	ARG	NE-CZ-NH1	-10.81	114.89	120.30
1	B	59	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	C	132	LEU	CA-CB-CG	10.58	139.64	115.30
1	A	73	ASP	CB-CG-OD2	-10.19	109.13	118.30
1	A	147	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	B	147	ARG	NE-CZ-NH1	-9.93	115.33	120.30
1	A	89	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	D	124	ASP	CB-CG-OD1	-9.68	109.58	118.30
1	A	73	ASP	CB-CG-OD1	9.39	126.75	118.30
1	A	66	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	C	66	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	D	78	LEU	CB-CG-CD2	-9.18	95.40	111.00
1	D	142	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	C	147	ARG	NE-CZ-NH1	-8.67	115.96	120.30
1	C	160	ARG	NE-CZ-NH2	8.57	124.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	LEU	CB-CG-CD2	-8.55	96.46	111.00
1	B	40	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	166	LEU	CB-CG-CD1	-8.00	97.41	111.00
1	A	109	ARG	NE-CZ-NH1	-7.95	116.33	120.30
1	B	130	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	D	136	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	160	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	D	73	ASP	CB-CG-OD1	7.72	125.25	118.30
1	D	76	LEU	N-CA-C	-7.62	90.42	111.00
1	B	166	LEU	CA-CB-CG	7.61	132.80	115.30
1	D	152	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	D	163	LEU	CB-CG-CD2	7.59	123.91	111.00
1	A	20	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	C	34	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	C	21	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	C	60	ILE	CG1-CB-CG2	-7.38	95.16	111.40
1	D	147	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	30	LEU	CA-CB-CG	7.28	132.04	115.30
1	B	71	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	A	160	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	C	4	LYS	CD-CE-NZ	-7.13	95.31	111.70
1	C	139	LEU	CB-CG-CD1	7.12	123.11	111.00
1	A	30	LEU	CB-CG-CD2	-7.08	98.96	111.00
1	B	165	ARG	NE-CZ-NH1	-6.99	116.81	120.30
1	B	32	ASP	CB-CG-OD1	-6.97	112.03	118.30
1	B	71	ASP	CB-CG-OD2	6.95	124.55	118.30
1	D	128	LYS	CD-CE-NZ	-6.93	95.75	111.70
1	D	20	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	119	LEU	CB-CG-CD1	-6.87	99.33	111.00
1	C	92	LEU	CB-CG-CD2	-6.83	99.38	111.00
1	A	132	LEU	CB-CG-CD1	-6.82	99.41	111.00
1	D	47	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	D	115	THR	N-CA-C	6.72	129.15	111.00
1	D	32	ASP	CB-CG-OD1	-6.65	112.32	118.30
1	D	117	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	61	GLU	OE1-CD-OE2	6.62	131.24	123.30
1	D	40	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	69	LEU	CB-CG-CD2	-6.55	99.86	111.00
1	B	30	LEU	CB-CG-CD1	-6.51	99.94	111.00
1	A	148	VAL	CB-CA-C	-6.46	99.13	111.40
1	D	65	VAL	CG1-CB-CG2	-6.36	100.73	110.90
1	D	100	LEU	CB-CG-CD2	6.35	121.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	21	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	92	LEU	CB-CG-CD1	-6.26	100.36	111.00
1	B	125	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	C	31	LEU	CB-CG-CD1	-6.21	100.45	111.00
1	D	60	ILE	CG1-CB-CG2	-6.18	97.81	111.40
1	B	10	LEU	CB-CG-CD1	-6.17	100.50	111.00
1	D	20	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	D	120	LEU	CB-CG-CD1	-6.09	100.64	111.00
1	C	136	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	124	ASP	N-CA-CB	-6.08	99.67	110.60
1	A	78	LEU	CB-CG-CD1	-6.03	100.75	111.00
1	C	89	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	C	148	VAL	CG1-CB-CG2	-5.94	101.40	110.90
1	B	111	THR	CA-CB-CG2	-5.89	104.15	112.40
1	A	147	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	71	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	D	165	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	D	38	GLU	CG-CD-OE1	-5.86	106.59	118.30
1	D	110	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	B	40	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	21	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	D	130	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	121	ALA	N-CA-CB	5.73	118.12	110.10
1	C	162	ILE	CG1-CB-CG2	5.70	123.94	111.40
1	B	92	LEU	CB-CG-CD2	5.70	120.69	111.00
1	B	141	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	C	89	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	26	LEU	CA-CB-CG	-5.59	102.45	115.30
1	B	116	VAL	N-CA-CB	5.59	123.79	111.50
1	A	154	ASN	C-N-CD	5.57	140.10	128.40
1	A	96	THR	CA-CB-CG2	-5.57	104.60	112.40
1	D	31	LEU	CB-CG-CD2	5.57	120.46	111.00
1	B	116	VAL	CA-CB-CG2	5.51	119.17	110.90
1	C	136	ARG	CG-CD-NE	-5.51	100.23	111.80
1	B	24	LYS	N-CA-CB	5.50	120.51	110.60
1	C	48	ILE	N-CA-C	-5.50	96.16	111.00
1	B	108	VAL	CG1-CB-CG2	-5.46	102.16	110.90
1	D	132	LEU	CA-CB-CG	5.46	127.86	115.30
1	B	121	ALA	CB-CA-C	-5.46	101.92	110.10
1	D	136	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	122	GLY	N-CA-C	5.43	126.67	113.10
1	C	141	ARG	NE-CZ-NH1	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	124	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	129	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	B	131	ALA	N-CA-CB	5.38	117.63	110.10
1	C	83	VAL	N-CA-C	5.37	125.51	111.00
1	C	99	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	D	142	ARG	CA-CB-CG	-5.35	101.64	113.40
1	A	164	SER	CA-CB-OG	-5.33	96.80	111.20
1	A	40	ARG	CB-CA-C	5.27	120.94	110.40
1	C	133	MET	CG-SD-CE	5.27	108.63	100.20
1	D	106	GLU	OE1-CD-OE2	5.27	129.62	123.30
1	D	21	ARG	NH1-CZ-NH2	5.26	125.19	119.40
1	C	153	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	139	LEU	CB-CG-CD1	5.22	119.87	111.00
1	A	125	ARG	NH1-CZ-NH2	5.20	125.11	119.40
1	C	24	LYS	CD-CE-NZ	5.19	123.65	111.70
1	A	61	GLU	CG-CD-OE1	-5.19	107.91	118.30
1	A	66	ARG	CD-NE-CZ	-5.18	116.34	123.60
1	C	22	LEU	CB-CG-CD1	5.18	119.80	111.00
1	C	110	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	58	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	66	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	63	ASP	CB-CA-C	5.14	120.68	110.40
1	D	108	VAL	CG1-CB-CG2	-5.14	102.68	110.90
1	D	66	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	D	32	ASP	CB-CG-OD2	5.12	122.90	118.30
1	C	130	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	C	58	ARG	CB-CA-C	5.10	120.60	110.40
1	B	89	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	7	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	165	ARG	CB-CA-C	5.09	120.59	110.40
1	A	26	LEU	CB-CA-C	-5.09	100.52	110.20
1	C	59	ARG	CB-CG-CD	5.07	124.79	111.60
1	B	146	MET	CB-CG-SD	-5.05	97.24	112.40
1	B	7	LEU	CB-CG-CD2	5.05	119.58	111.00
1	D	36	ALA	N-CA-CB	5.02	117.12	110.10
1	C	62	GLU	CG-CD-OE1	-5.01	108.27	118.30
1	A	51	THR	N-CA-C	5.00	124.50	111.00

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 ⓘ

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	110	0
1	B	1229	0	1282	114	1
1	C	1157	0	1202	123	1
1	D	1226	0	1275	110	1
2	A	1	0	0	0	0
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	31	2
5	B	85	0	0	47	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	51	0	0	38	1
5	D	64	0	0	33	1
All	All	5152	0	5015	457	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 46.

All (457) 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
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:D:121:ALA:C	1:D:123:PRO:HD2	1.66	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:121:ALA:C	1:D:123:PRO:CD	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:121:ALA:C	5:B:401:HOH:O	2.21	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:55:GLN:H	1:A:55:GLN:CD	1.97	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:129:TYR:CD1	1:D:129:TYR:C	2.66	0.66
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
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:C:51:THR:C	5:C:274:HOH:O	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:17:THR:O	1:D:21:ARG:HG3	1.99	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:D:106:GLU:O	1:D:110:ARG:HB2	2.00	0.60
4:C:182:ADP:O3'	4:D:183:ADP:O3'	2.07	0.60
1:D:134:ALA:O	5:D:239:HOH:O	2.17	0.59
1:D:102:ILE:HD11	1:D:106:GLU:CB	2.31	0.59
1:D:72:HIS:NE2	1:D:74:GLY:HA3	2.18	0.59
1:D:88:VAL:O	1:D:89:ARG:C	2.39	0.58
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:D:161:HIS:C	1:D:161:HIS:CD2	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:46:ALA:O	1:A:48:ILE:N	2.38	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: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:B:57:PHE:C	1:B:57:PHE:CD2	2.80	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
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:D:120:LEU:O	1:D:121:ALA:C	2.45	0.55
1:A:114:ASN:C	5:A:423:HOH:O	2.45	0.55
1:D:17:THR:OG1	4:D:183:ADP:H2'	2.07	0.55
1:D:112:GLY:C	1:D:114:ASN:N	2.61	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:C:165:ARG:O	1:C:166:LEU:C	2.46	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:B:79:GLY:C	5:B:227:HOH:O	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ARG:HG2	5:C:420:HOH:O	2.07	0.53
1:B:147:ARG:O	1:B:147:ARG:CG	2.54	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: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: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:D:88:VAL:O	1:D:90:ALA:N	2.42	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:110:ARG:HB3	4:A:180:ADP:O4'	2.08	0.52
1:B:150:THR:O	1:B:151:ASN:C	2.48	0.52
1:C:26:LEU:HA	5:C:219:HOH:O	2.09	0.51
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: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:79:GLY:O	1:C:80:GLY:C	2.50	0.50
1:C:104:ALA:HA	1:C:129:TYR:CE1	2.46	0.50
1:D:26:LEU:O	1:D:27:GLY:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:21:ARG:HB2	1:D:159:VAL:HG21	1.94	0.49
1:A:155:PRO:O	1:A:156:GLY:C	2.50	0.49
1:C:12:GLY:O	1:C:13:SER:C	2.50	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: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
4:A:180:ADP:HO2'	4:B:181:ADP:HO3'	1.61	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
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: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:A:136:ARG:O	1:A:137:ALA:C	2.51	0.47
1:C:157:ALA:HB2	5:C:411:HOH:O	1.80	0.47
1:C:162:ILE:O	1:C:163:LEU:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:129:TYR:C	1:D:129:TYR:HD1	2.14	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: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:A:102:ILE:O	1:A:102:ILE:CG2	2.63	0.46
1:D:43:ARG:NH2	1:D:52:ASP:OD1	2.45	0.46
1:C:31:LEU:CD2	1:C:32:ASP:N	2.78	0.46
1:B:54:GLU:C	1:B:56:GLU:H	2.16	0.46
1:A:153:ARG:NH2	1:A:161:HIS:ND1	2.63	0.46
1:B:30:LEU:HA	1:B:30:LEU:HD12	1.60	0.46
1:B:131:ALA:O	1:B:132:LEU:C	2.54	0.46
1:B:152:ARG:C	5:B:250:HOH:O	2.54	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
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: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: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: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:C:64:VAL:O	1:C:65:VAL:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:108:VAL:O	1:A:108:VAL:HG12	2.16	0.44
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:C:165:ARG:C	5:C:320:HOH:O	2.55	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: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:B:6:VAL:HA	1:B:76:LEU:O	2.18	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: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:B:149:ASP:OD1	1:B:151:ASN:ND2	2.33	0.43
1:B:111:THR:HB	1:B:117:ARG:HD3	2.01	0.43
1:D:124:ASP:CG	5:D:471:HOH:O	2.57	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: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:D:123:PRO:HB2	1:D:128:LYS:HZ3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:37:ILE:O	1:A:41:THR:CG2	2.67	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:D:162:ILE:O	1:D:166:LEU:HG	2.20	0.42
1:A:64:VAL:O	1:A:64:VAL:CG1	2.67	0.41
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:61:GLU:CD	1:A:82:ALA:HB2	2.40	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:B:18:ILE:O	1:B:22:LEU:CB	2.69	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:C:66:ARG:NH2	1:C:87:GLY:C	2.73	0.41
1:D:67:ALA:O	1:D:68:ALA:C	2.58	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:14:GLY:O	1:B:15:LYS:C	2.59	0.41
1:B:24:LYS:NZ	5:B:256:HOH:O	2.25	0.41
1:B:122:GLY:HA3	1:B:123:PRO:HD3	1.93	0.41
1:D:124:ASP:C	1:D:124:ASP:OD1	2.58	0.41
1:A:99:TYR:CE1	1:A:140:TYR:HB3	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:55:GLN:CD	1:B:55:GLN:H	2.25	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:B:146:MET:HB2	1:B:146:MET:HE2	1.33	0.40
1:C:58:ARG:NH2	1:C:81:GLY:HA3	2.37	0.40
1:C:24:LYS:C	1:C:26:LEU:H	2.25	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	152/176 (86%)	132 (87%)	14 (9%)	6 (4%)	3	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	163/176 (93%)	133 (82%)	17 (10%)	13 (8%)	1	2
1	C	151/176 (86%)	129 (85%)	14 (9%)	8 (5%)	2	6
1	D	163/176 (93%)	136 (83%)	12 (7%)	15 (9%)	1	1
All	All	629/704 (89%)	530 (84%)	57 (9%)	42 (7%)	1	3

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

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Mol	Chain	Res	Type
1	D	122	GLY
1	B	18	ILE
1	D	121	ALA
1	D	124	ASP
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 ⓘ

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%)	97 (84%)	19 (16%)	2	7
1	B	123/132 (93%)	108 (88%)	15 (12%)	5	15
1	C	115/132 (87%)	93 (81%)	22 (19%)	1	4
1	D	122/132 (92%)	104 (85%)	18 (15%)	3	9
All	All	476/528 (90%)	402 (84%)	74 (16%)	2	8

All (74) 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	52	ASP
1	A	54	GLU
1	A	55	GLN
1	A	59	ARG
1	A	63	ASP
1	A	89	ARG
1	A	101	GLU

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Mol	Chain	Res	Type
1	A	102	ILE
1	A	128	LYS
1	A	130	ARG
1	A	135	LYS
1	A	154	ASN
1	A	165	ARG
1	A	166	LEU
1	B	20	ARG
1	B	21	ARG
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	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	59	ARG
1	C	63	ASP
1	C	84	THR
1	C	125	ARG
1	C	130	ARG
1	C	132	LEU
1	C	136	ARG
1	C	151	ASN
1	C	153	ARG

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Mol	Chain	Res	Type
1	C	160	ARG
1	C	166	LEU
1	D	15	LYS
1	D	16	SER
1	D	21	ARG
1	D	22	LEU
1	D	24	LYS
1	D	39	GLN
1	D	45	ILE
1	D	55	GLN
1	D	59	ARG
1	D	71	ASP
1	D	99	TYR
1	D	102	ILE
1	D	127	GLU
1	D	129	TYR
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	B	39	GLN
1	B	114	ASN
1	C	151	ASN
1	C	161	HIS
1	D	39	GLN
1	D	55	GLN

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 (i)

There are no monosaccharides 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	24,29,29	0.95	1 (4%)	29,45,45	2.61	13 (44%)
4	ADP	B	181	2	24,29,29	1.04	2 (8%)	29,45,45	2.67	9 (31%)
4	ADP	A	180	2	24,29,29	1.16	2 (8%)	29,45,45	2.54	13 (44%)
4	ADP	D	183	2	24,29,29	0.74	0	29,45,45	2.17	8 (27%)

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	-	3/12/32/32	0/3/3/3
4	ADP	B	181	2	-	3/12/32/32	0/3/3/3
4	ADP	A	180	2	-	5/12/32/32	0/3/3/3
4	ADP	D	183	2	-	5/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	180	ADP	C2'-C1'	-3.04	1.49	1.53
4	B	181	ADP	C8-N7	2.46	1.39	1.34
4	B	181	ADP	C2-N3	2.12	1.35	1.32
4	A	180	ADP	C5-N7	-2.06	1.32	1.39
4	C	182	ADP	PB-O3B	-2.03	1.47	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	181	ADP	C4-C5-N7	-8.25	100.81	109.40
4	D	183	ADP	N3-C2-N1	-7.09	117.60	128.68
4	B	181	ADP	C5-C6-N6	6.07	129.57	120.35
4	C	182	ADP	N3-C2-N1	-5.87	119.51	128.68
4	C	182	ADP	C2'-C3'-C4'	5.58	113.48	102.64
4	A	180	ADP	O4'-C1'-C2'	-5.20	99.33	106.93
4	A	180	ADP	C4-C5-N7	-4.76	104.44	109.40
4	A	180	ADP	O4'-C4'-C3'	-4.55	96.12	105.11
4	C	182	ADP	C1'-N9-C4	-4.45	118.82	126.64
4	A	180	ADP	PA-O3A-PB	-4.32	118.02	132.83
4	C	182	ADP	O2A-PA-O1A	4.15	132.77	112.24
4	B	181	ADP	O2'-C2'-C3'	-4.05	98.72	111.82
4	C	182	ADP	C3'-C2'-C1'	-3.99	94.98	100.98
4	A	180	ADP	O4'-C4'-C5'	-3.90	96.54	109.37
4	B	181	ADP	N6-C6-N1	-3.88	110.52	118.57
4	A	180	ADP	N3-C2-N1	-3.81	122.73	128.68
4	D	183	ADP	PA-O3A-PB	-3.69	120.16	132.83
4	D	183	ADP	O2'-C2'-C3'	-3.68	99.93	111.82
4	C	182	ADP	C2-N1-C6	3.66	125.02	118.75
4	A	180	ADP	C2'-C3'-C4'	3.57	109.58	102.64
4	A	180	ADP	O2B-PB-O1B	3.42	124.07	110.68
4	A	180	ADP	O3'-C3'-C2'	-3.28	101.20	111.82
4	C	182	ADP	O4'-C4'-C3'	-3.09	99.00	105.11
4	B	181	ADP	O3'-C3'-C2'	-3.07	101.88	111.82
4	D	183	ADP	C4-C5-N7	-2.93	106.35	109.40
4	B	181	ADP	O5'-C5'-C4'	-2.92	98.94	108.99
4	C	182	ADP	C4-C5-N7	-2.91	106.36	109.40
4	D	183	ADP	O4'-C1'-C2'	-2.87	102.74	106.93
4	D	183	ADP	O3'-C3'-C4'	-2.85	102.82	111.05
4	B	181	ADP	O3A-PB-O1B	-2.78	95.74	111.19
4	D	183	ADP	C3'-C2'-C1'	2.66	104.98	100.98
4	A	180	ADP	O5'-C5'-C4'	-2.55	100.23	108.99
4	B	181	ADP	O2A-PA-O1A	2.49	124.54	112.24
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	C	182	ADP	PA-O5'-C5'	2.44	136.01	121.68
4	A	180	ADP	O3B-PB-O1B	-2.33	101.56	110.68
4	D	183	ADP	C5-C6-N6	2.27	123.81	120.35
4	C	182	ADP	O4'-C1'-C2'	2.26	110.23	106.93
4	A	180	ADP	O2A-PA-O1A	2.22	123.20	112.24
4	A	180	ADP	C3'-C2'-C1'	-2.17	97.71	100.98
4	C	182	ADP	O2B-PB-O1B	2.17	119.17	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	182	ADP	O2B-PB-O3A	2.16	111.89	104.64

There are no chirality outliers.

All (16) 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	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-O1A
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	C5'-O5'-PA-O3A
4	A	180	ADP	C5'-O5'-PA-O2A
4	C	182	ADP	C5'-O5'-PA-O2A
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 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 C 182

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 181

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 180

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 183

Bond lengths

Bond angles

Torsions

Rings
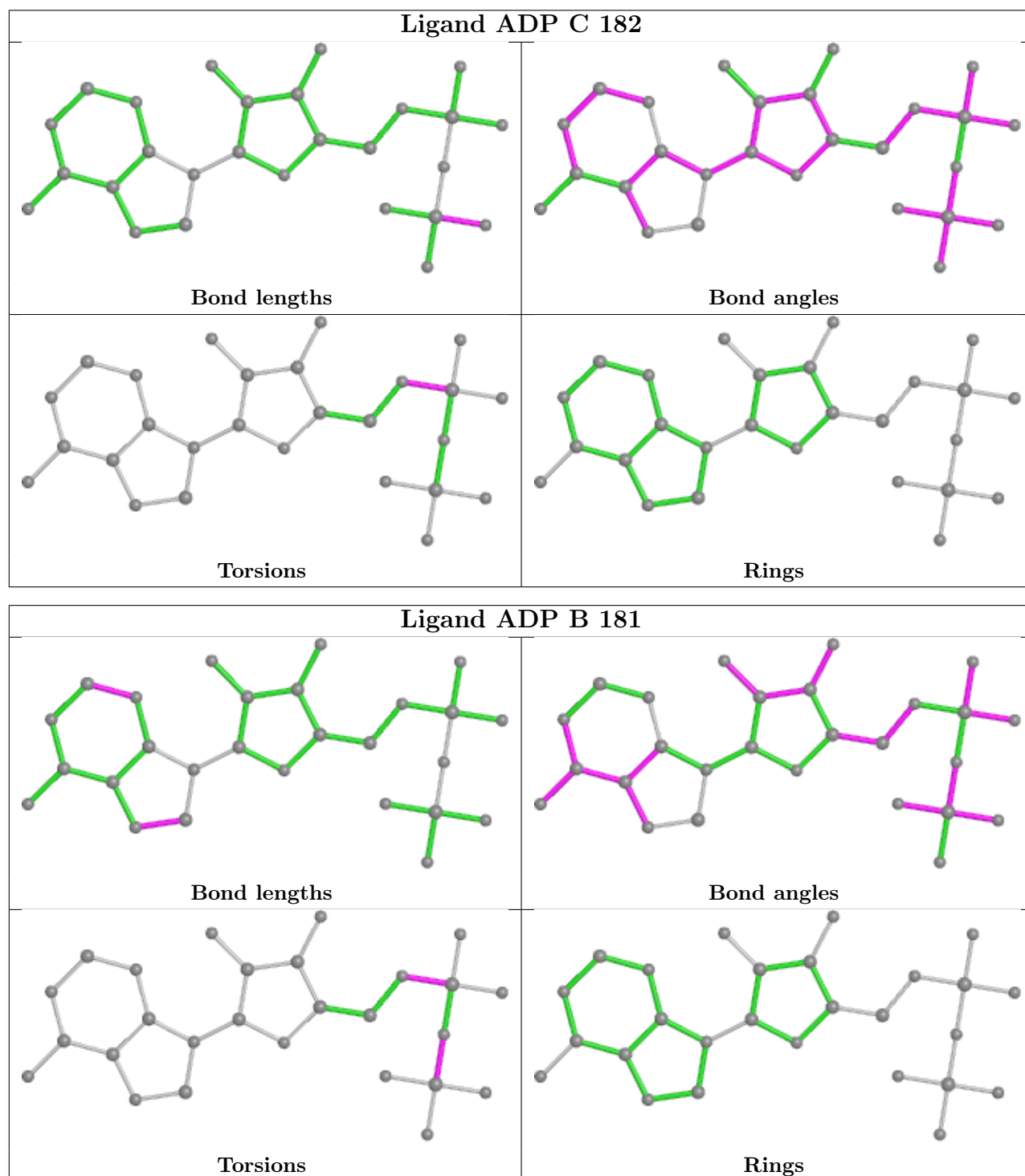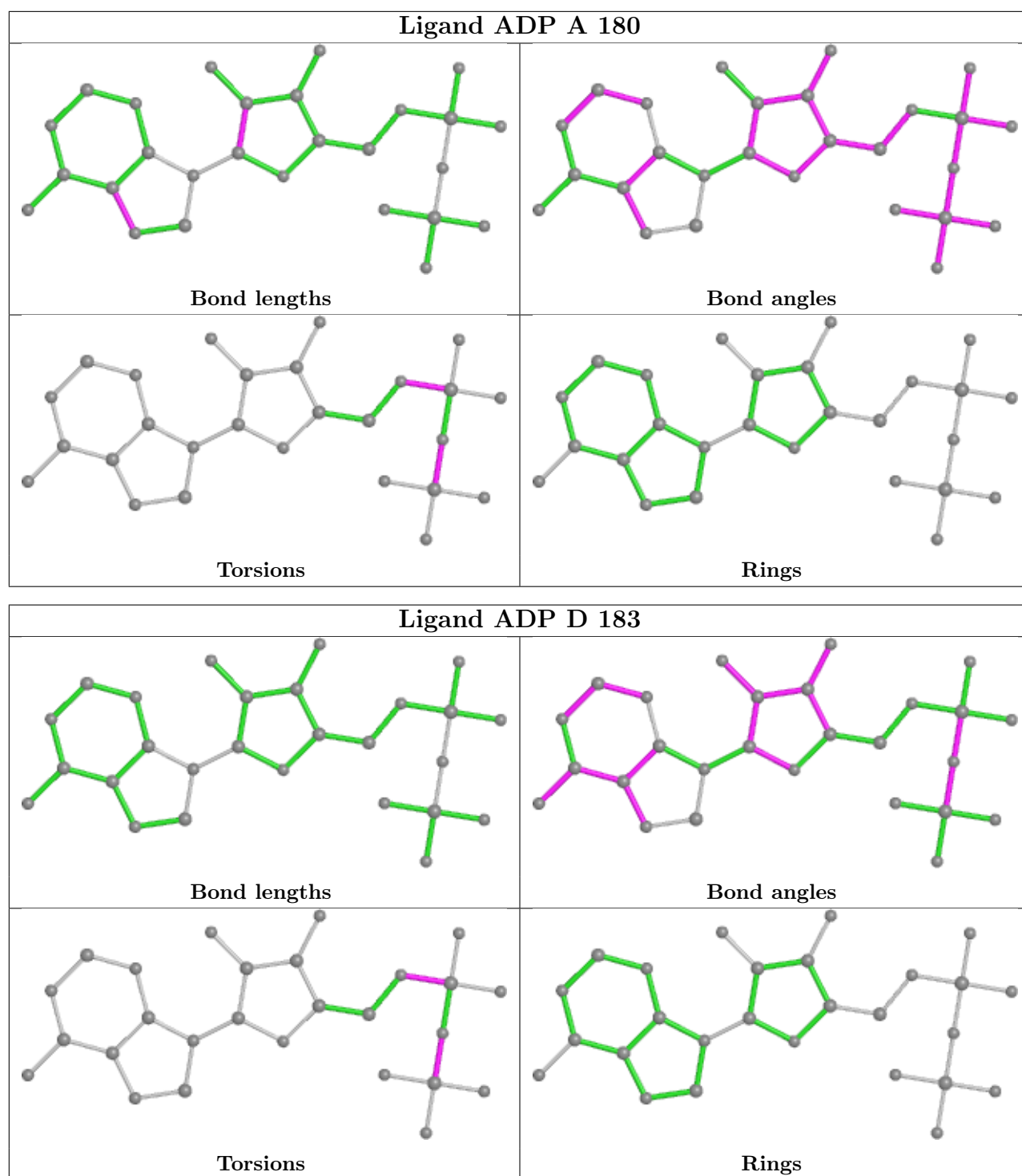
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	156/176 (88%)	-0.45	0	100	100	12, 32, 53, 68	0
1	B	165/176 (93%)	-0.50	0	100	100	9, 28, 46, 62	0
1	C	155/176 (88%)	-0.35	0	100	100	18, 34, 61, 83	0
1	D	165/176 (93%)	-0.34	1 (0%)	89	86	20, 36, 54, 68	0
All	All	641/704 (91%)	-0.41	1 (0%)	95	94	9, 33, 53, 83	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	ASN	2.9

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 monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
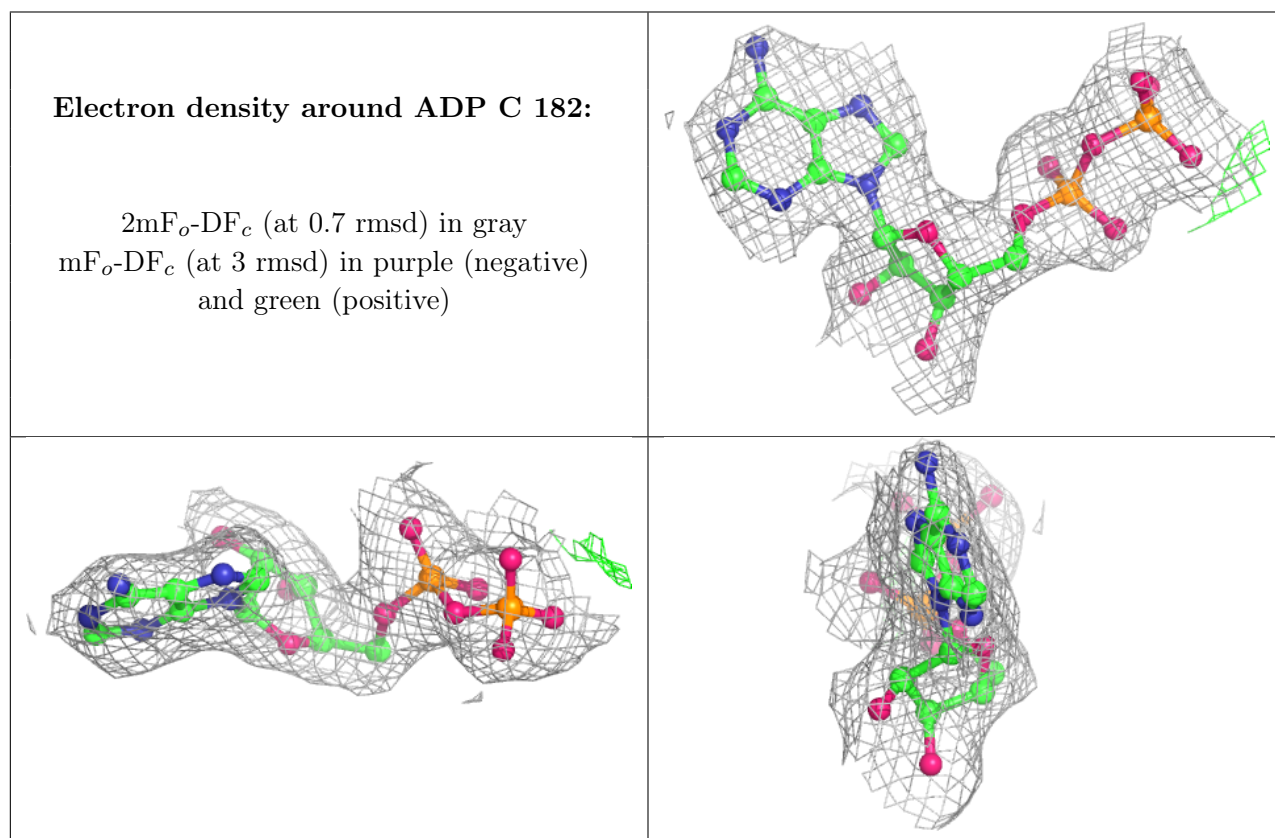
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	C	202	1/1	0.79	0.21	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
2	MG	D	208	1/1	0.89	0.21	41,41,41,41	0
2	MG	A	190	1/1	0.90	0.23	22,22,22,22	0
3	CL	A	193	1/1	0.91	0.09	46,46,46,46	0
2	MG	B	196	1/1	0.92	0.20	15,15,15,15	0
3	CL	D	211	1/1	0.95	0.12	34,34,34,34	0
4	ADP	C	182	27/27	0.97	0.13	7,29,43,54	0
4	ADP	A	180	27/27	0.98	0.11	10,16,25,32	0
4	ADP	D	183	27/27	0.98	0.13	17,33,49,52	0
3	CL	B	199	1/1	0.99	0.10	26,26,26,26	0
4	ADP	B	181	27/27	0.99	0.13	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.
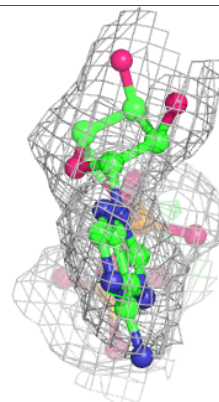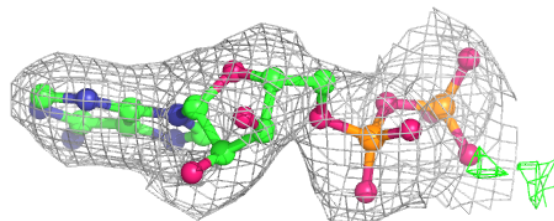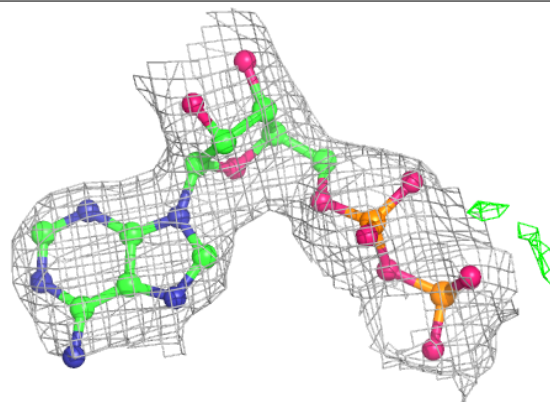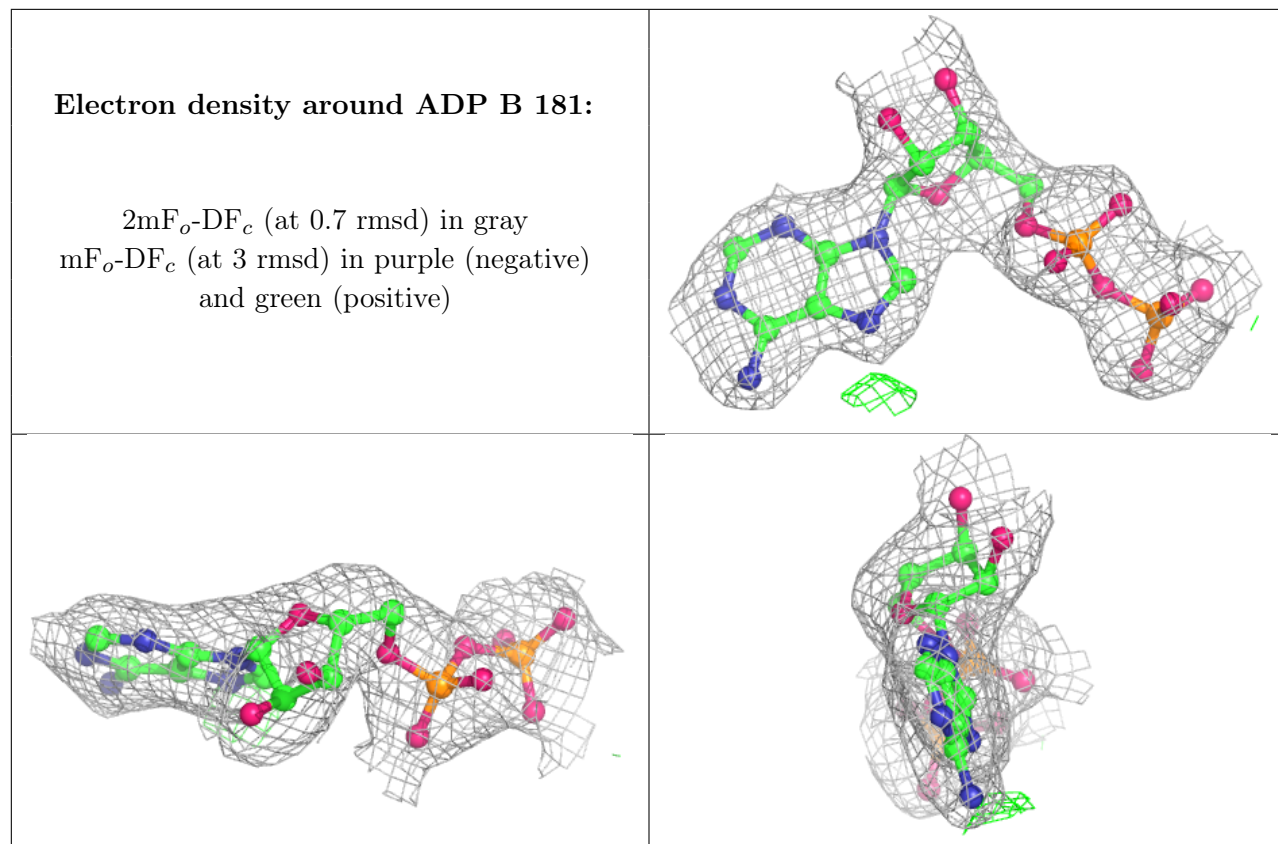

Electron density around ADP C 182:

$2mF_o$-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 A 180:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
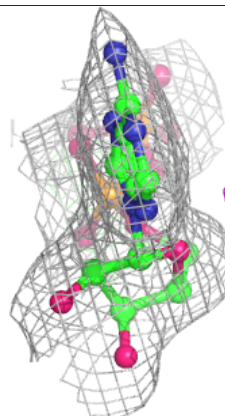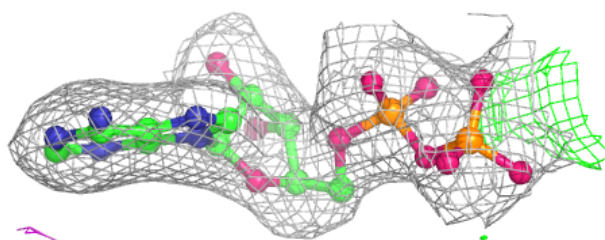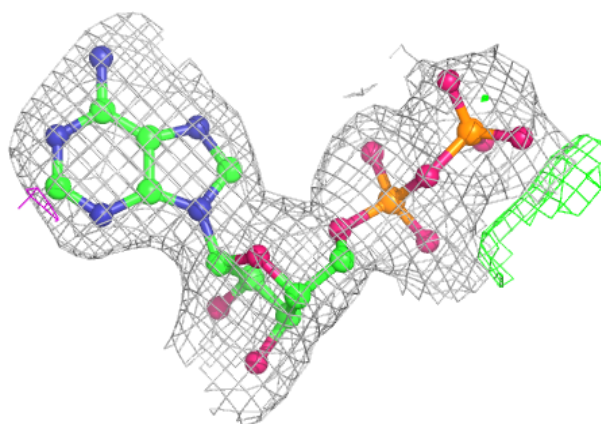
Electron density around ADP D 183:

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

Electron density around ADP B 181:

$2mF_o$-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.