



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:15 pm BST

PDB ID : 1XNJ
Title : APS complex of human PAPS synthetase 1
Authors : Harjes, S.; Bayer, P.; Scheidig, A.J.
Deposited on : 2004-10-05
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

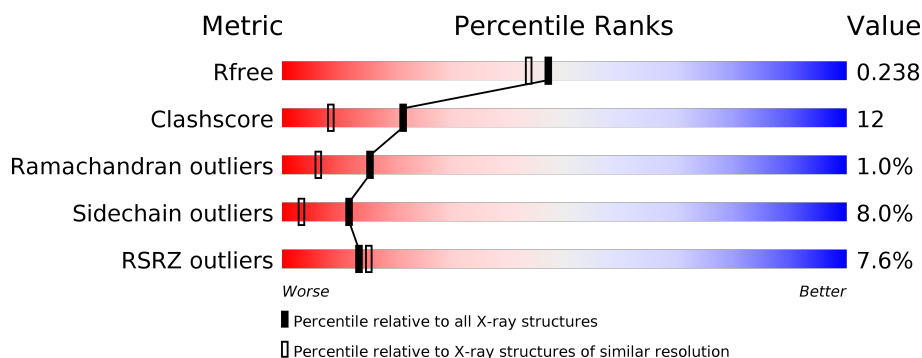
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	630	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>23%</div> <div>• • 11%</div> </div> </div>
1	B	630	<div> <div>8%</div> <div> <div></div> <div>57%</div> <div>29%</div> <div>6% • 6%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10000 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 Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	590	Total	C	N	O	S	0	4	0
			4717	2989	830	867	31			
1	A	562	Total	C	N	O	S	0	8	0
			4508	2856	793	827	32			

There are 14 discrepancies between the modelled and reference sequences:

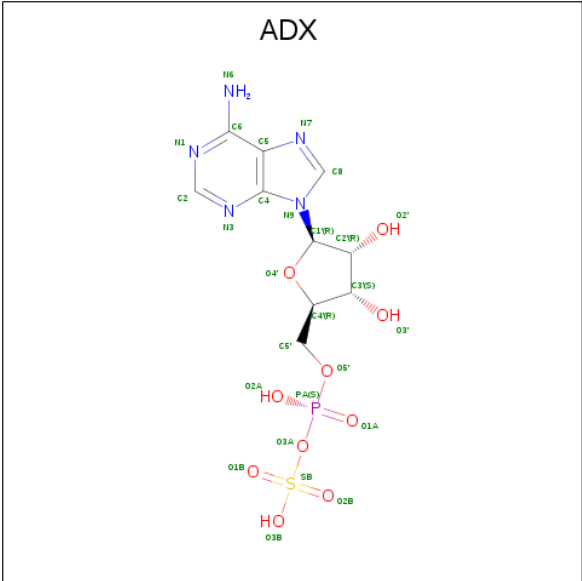
Chain	Residue	Modelled	Actual	Comment	Reference
B	416	SER	PHE	CONFLICT	UNP O43252
B	625	HIS	-	EXPRESSION TAG	UNP O43252
B	626	HIS	-	EXPRESSION TAG	UNP O43252
B	627	HIS	-	EXPRESSION TAG	UNP O43252
B	628	HIS	-	EXPRESSION TAG	UNP O43252
B	629	HIS	-	EXPRESSION TAG	UNP O43252
B	630	HIS	-	EXPRESSION TAG	UNP O43252
A	416	SER	PHE	CONFLICT	UNP O43252
A	625	HIS	-	EXPRESSION TAG	UNP O43252
A	626	HIS	-	EXPRESSION TAG	UNP O43252
A	627	HIS	-	EXPRESSION TAG	UNP O43252
A	628	HIS	-	EXPRESSION TAG	UNP O43252
A	629	HIS	-	EXPRESSION TAG	UNP O43252
A	630	HIS	-	EXPRESSION TAG	UNP O43252

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is ADENOSINE-5'-PHOSPHOSULFATE (three-letter code: ADX) (formula: C₁₀H₁₄N₅O₁₀PS).



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

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

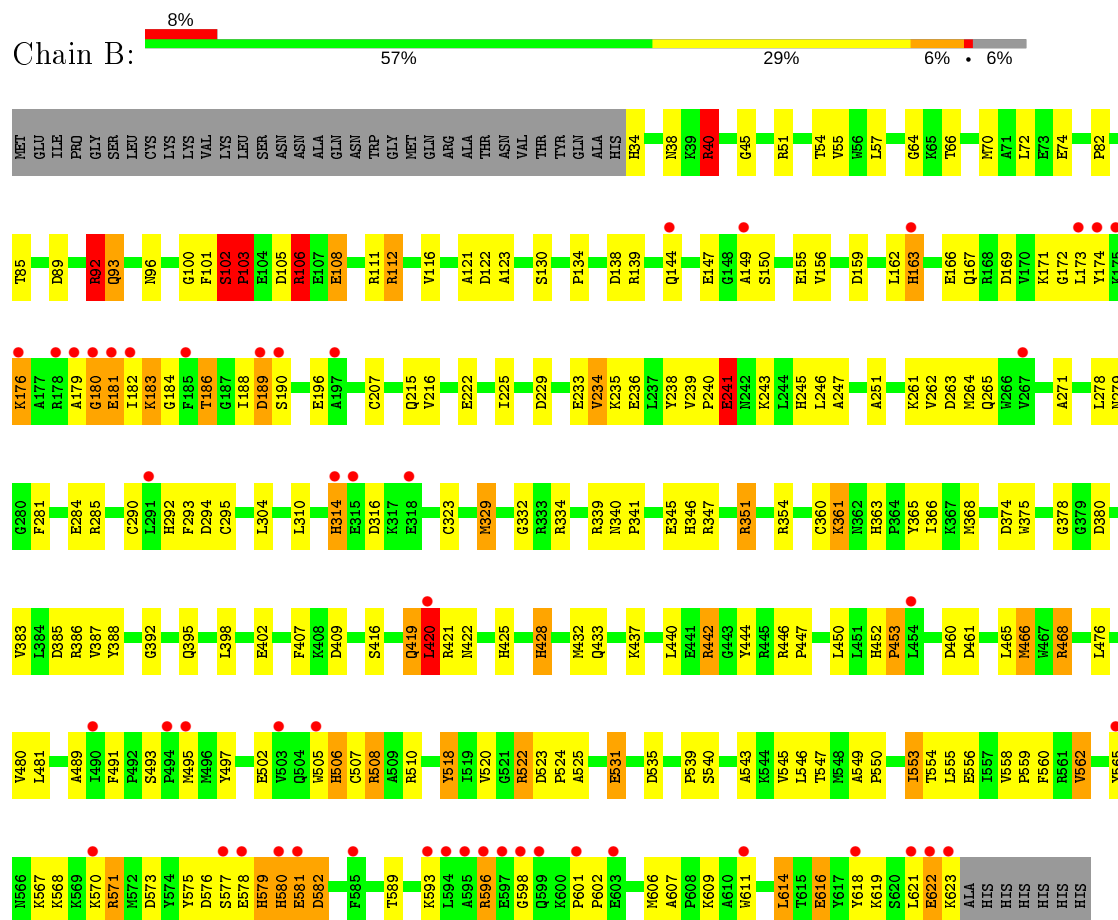
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	324	Total	O	0	0
			324	324		
4	A	343	Total	O	0	0
			343	343		

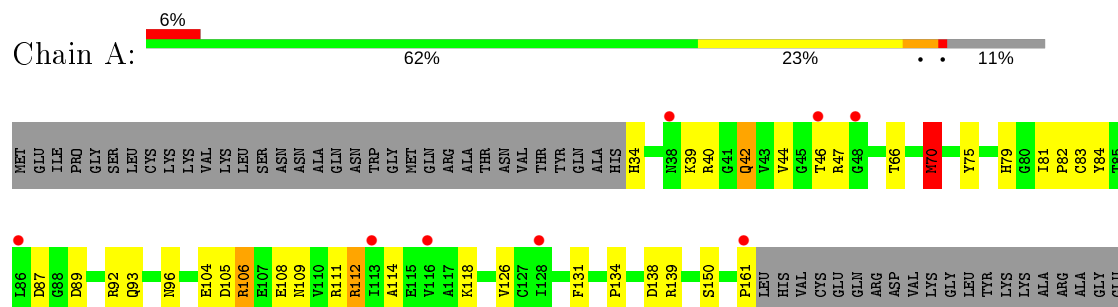
3 Residue-property plots [i](#)

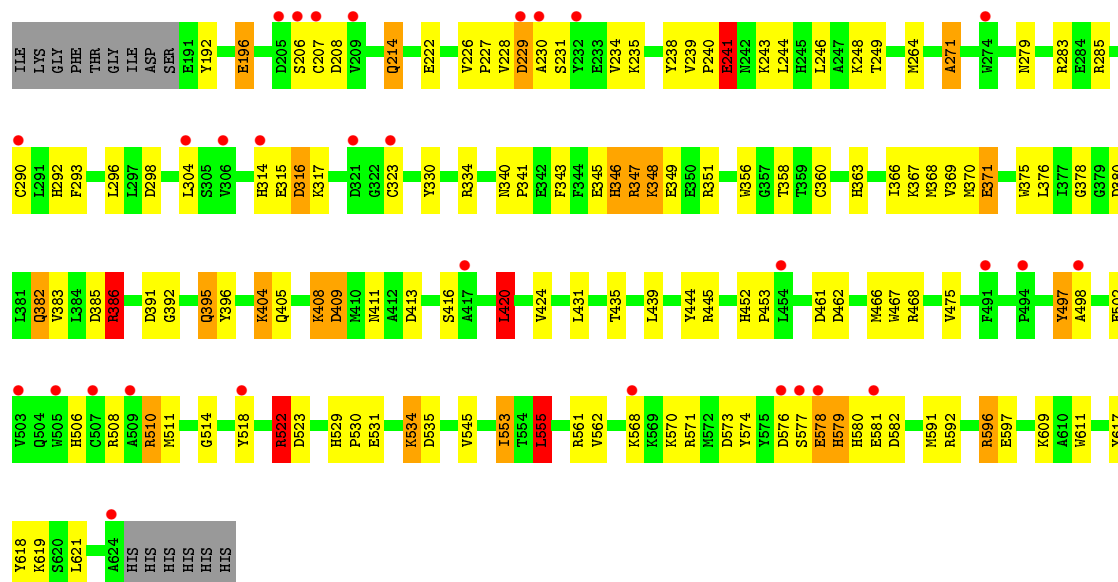
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1



- Molecule 1: Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.50Å 82.50Å 133.00Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	129.10 – 1.98 38.01 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.0 (129.10-1.98) 97.0 (38.01-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.184 , 0.239 0.191 , 0.238	Depositor DCC
R_{free} test set	5581 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10000	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.64	52/4663 (1.1%)	1.37	53/6321 (0.8%)
1	B	1.66	50/4846 (1.0%)	1.44	62/6563 (0.9%)
All	All	1.65	102/9509 (1.1%)	1.41	115/12884 (0.9%)

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	2
1	B	0	2
All	All	0	4

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	GLU	CD-OE1	10.01	1.36	1.25
1	B	518	TYR	CD1-CE1	-8.64	1.26	1.39
1	A	238	TYR	CE1-CZ	-8.50	1.27	1.38
1	B	518	TYR	CE2-CZ	-8.16	1.27	1.38
1	B	238	TYR	CD2-CE2	-7.94	1.27	1.39
1	B	55	VAL	CB-CG1	-7.85	1.36	1.52
1	B	222	GLU	CD-OE2	7.73	1.34	1.25
1	A	592	ARG	NE-CZ	7.34	1.42	1.33
1	B	505	TRP	CE3-CZ3	-7.32	1.26	1.38
1	B	234	VAL	CB-CG2	-7.26	1.37	1.52
1	A	518	TYR	CZ-OH	-7.24	1.25	1.37
1	B	518	TYR	CG-CD1	-7.12	1.29	1.39
1	A	611	TRP	CB-CG	-7.10	1.37	1.50
1	B	40	ARG	CG-CD	7.04	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ARG	NE-CZ	-7.03	1.24	1.33
1	B	241	GLU	CD-OE1	7.01	1.33	1.25
1	A	518	TYR	CE2-CZ	-6.97	1.29	1.38
1	A	396	TYR	CG-CD1	-6.84	1.30	1.39
1	A	522	ARG	CG-CD	6.83	1.69	1.51
1	B	40	ARG	CB-CG	6.79	1.70	1.52
1	A	368	MET	CG-SD	6.77	1.98	1.81
1	A	349	GLU	CG-CD	6.71	1.62	1.51
1	B	407	PHE	CD2-CE2	6.70	1.52	1.39
1	A	118	LYS	CE-NZ	6.68	1.65	1.49
1	B	531	GLU	CG-CD	6.66	1.61	1.51
1	A	574	TYR	CD1-CE1	-6.63	1.29	1.39
1	A	315	GLU	CD-OE1	6.53	1.32	1.25
1	A	371	GLU	CD-OE2	6.42	1.32	1.25
1	B	419	GLN	CG-CD	-6.40	1.36	1.51
1	B	238	TYR	CE1-CZ	-6.40	1.30	1.38
1	B	293	PHE	CE2-CZ	-6.37	1.25	1.37
1	A	408	LYS	CD-CE	6.34	1.67	1.51
1	A	345	GLU	CD-OE2	6.32	1.32	1.25
1	B	347	ARG	CZ-NH1	6.24	1.41	1.33
1	A	241	GLU	CD-OE1	6.22	1.32	1.25
1	B	345	GLU	CD-OE2	6.20	1.32	1.25
1	B	121	ALA	CA-CB	-6.14	1.39	1.52
1	B	497	TYR	CG-CD1	-6.01	1.31	1.39
1	A	617	TYR	CE1-CZ	-6.00	1.30	1.38
1	B	238	TYR	CD1-CE1	-6.00	1.30	1.39
1	A	104	GLU	CD-OE1	5.99	1.32	1.25
1	B	480	VAL	CB-CG2	5.99	1.65	1.52
1	A	238	TYR	CG-CD2	-5.99	1.31	1.39
1	A	404	LYS	CE-NZ	5.96	1.64	1.49
1	A	444	TYR	CD2-CE2	5.96	1.48	1.39
1	B	155	GLU	CG-CD	5.89	1.60	1.51
1	A	424	VAL	CB-CG2	-5.86	1.40	1.52
1	A	534	LYS	CD-CE	5.81	1.65	1.51
1	A	522	ARG	CB-CG	5.77	1.68	1.52
1	B	108	GLU	CG-CD	5.76	1.60	1.51
1	B	262	VAL	C-O	-5.73	1.12	1.23
1	A	545	VAL	CB-CG1	-5.71	1.40	1.52
1	B	74	GLU	CD-OE1	5.71	1.31	1.25
1	B	361	LYS	CD-CE	5.68	1.65	1.51
1	B	284	GLU	CD-OE1	-5.68	1.19	1.25
1	A	617	TYR	CD2-CE2	-5.61	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	236	GLU	CD-OE1	-5.58	1.19	1.25
1	B	329	MET	SD-CE	5.51	2.08	1.77
1	B	556	GLU	CD-OE2	5.49	1.31	1.25
1	B	442	ARG	CZ-NH1	5.47	1.40	1.33
1	B	89	ASP	CB-CG	5.42	1.63	1.51
1	A	518	TYR	CG-CD1	-5.42	1.32	1.39
1	A	249	THR	CB-CG2	5.42	1.70	1.52
1	A	562	VAL	CB-CG2	-5.40	1.41	1.52
1	B	453	PRO	CA-CB	5.40	1.64	1.53
1	A	467	TRP	CB-CG	-5.36	1.40	1.50
1	B	428	HIS	CA-CB	-5.36	1.42	1.53
1	B	432	MET	CG-SD	-5.36	1.67	1.81
1	B	540	SER	N-CA	-5.34	1.35	1.46
1	A	234	VAL	C-O	-5.32	1.13	1.23
1	A	514	GLY	C-O	-5.29	1.15	1.23
1	A	382	GLN	CG-CD	5.29	1.63	1.51
1	A	345	GLU	CG-CD	5.28	1.59	1.51
1	A	92	ARG	CZ-NH1	5.28	1.40	1.33
1	A	114	ALA	CA-CB	-5.26	1.41	1.52
1	A	70	MET	SD-CE	5.25	2.07	1.77
1	A	475	VAL	CB-CG2	-5.25	1.41	1.52
1	B	616	GLU	CG-CD	5.24	1.59	1.51
1	A	244	LEU	C-O	5.23	1.33	1.23
1	A	395	GLN	CG-CD	5.21	1.63	1.51
1	B	365	TYR	CD2-CE2	-5.20	1.31	1.39
1	B	614	LEU	C-O	5.19	1.33	1.23
1	A	617	TYR	CG-CD1	-5.19	1.32	1.39
1	B	93	GLN	CB-CG	5.17	1.66	1.52
1	A	271	ALA	CA-CB	-5.17	1.41	1.52
1	B	285	ARG	NE-CZ	-5.17	1.26	1.33
1	A	497	TYR	CE1-CZ	-5.14	1.31	1.38
1	A	618	TYR	CE1-CZ	-5.12	1.31	1.38
1	A	349	GLU	CD-OE1	-5.12	1.20	1.25
1	B	290	CYS	CB-SG	-5.12	1.73	1.81
1	B	402	GLU	CD-OE1	5.12	1.31	1.25
1	B	562	VAL	CB-CG2	-5.10	1.42	1.52
1	A	241	GLU	CD-OE2	5.10	1.31	1.25
1	A	347	ARG	CZ-NH1	5.10	1.39	1.33
1	B	147	GLU	CD-OE2	5.04	1.31	1.25
1	B	433	GLN	CA-C	-5.04	1.39	1.52
1	A	619	LYS	CE-NZ	5.04	1.61	1.49
1	B	281	PHE	CD2-CE2	5.03	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	LYS	CA-C	-5.03	1.39	1.52
1	A	131	PHE	CD1-CE1	-5.02	1.29	1.39
1	A	334	ARG	C-O	-5.01	1.13	1.23
1	B	262	VAL	CB-CG1	-5.01	1.42	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	MET	CG-SD-CE	-10.90	82.75	100.20
1	B	468	ARG	NE-CZ-NH1	-10.80	114.90	120.30
1	B	92	ARG	NE-CZ-NH2	10.01	125.30	120.30
1	B	576	ASP	CB-CG-OD2	9.97	127.27	118.30
1	B	40	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	A	523	ASP	CB-CG-OD2	9.61	126.95	118.30
1	B	316	ASP	CB-CG-OD2	9.53	126.88	118.30
1	B	139	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	B	345	GLU	OE1-CD-OE2	9.41	134.59	123.30
1	B	347	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	522	ARG	NE-CZ-NH2	9.31	124.95	120.30
1	B	159	ASP	CB-CG-OD2	9.30	126.67	118.30
1	B	122	ASP	CB-CG-OD2	9.24	126.62	118.30
1	A	112	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	A	316	ASP	CB-CG-OD2	9.17	126.55	118.30
1	A	404	LYS	CD-CE-NZ	8.89	132.15	111.70
1	B	189	ASP	CB-CG-OD2	8.77	126.20	118.30
1	A	391	ASP	CB-CG-OD2	8.61	126.05	118.30
1	A	468	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	112	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	B	334	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	B	40	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	B	571	ARG	NE-CZ-NH1	-8.27	116.17	120.30
1	A	334	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	B	106	ARG	CG-CD-NE	8.26	129.14	111.80
1	B	138	ASP	CB-CG-OD2	8.23	125.71	118.30
1	B	112	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	385	ASP	CB-CG-OD2	8.03	125.53	118.30
1	A	592	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	A	573	ASP	CB-CG-OD2	7.91	125.42	118.30
1	A	347	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	B	106	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	A	92	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	B	264	MET	CG-SD-CE	-7.49	88.22	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ASP	CB-CG-OD2	7.45	125.01	118.30
1	B	111	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	B	420	LEU	CB-CG-CD1	7.37	123.53	111.00
1	B	409	ASP	CB-CG-OD2	7.35	124.91	118.30
1	B	508	ARG	NE-CZ-NH2	7.31	123.96	120.30
1	A	462	ASP	CB-CG-OD2	7.31	124.88	118.30
1	A	380	ASP	CB-CG-OD2	7.25	124.83	118.30
1	B	263	ASP	CB-CG-OD2	7.19	124.77	118.30
1	B	354	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	339	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	B	531	GLU	OE1-CD-OE2	-7.00	114.90	123.30
1	A	420	LEU	CA-CB-CG	6.93	131.24	115.30
1	A	138	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	510	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	A	87	ASP	CB-CG-OD2	6.85	124.47	118.30
1	B	508	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	A	323[A]	CYS	CA-CB-SG	6.79	126.23	114.00
1	A	323[B]	CYS	CA-CB-SG	6.79	126.23	114.00
1	B	368	MET	CG-SD-CE	6.72	110.95	100.20
1	A	285	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	105	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	461	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	385	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	380	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	420	LEU	CB-CG-CD1	6.47	122.00	111.00
1	A	576	ASP	CB-CG-OD2	6.43	124.08	118.30
1	A	105	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	339	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	A	386	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	298	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	460	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	118	LYS	CD-CE-NZ	6.21	125.99	111.70
1	B	421	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	A	296	LEU	CB-CG-CD1	-6.15	100.54	111.00
1	A	347	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	229	ASP	CB-CG-OD2	6.06	123.76	118.30
1	B	573	ASP	CB-CG-OD2	6.05	123.75	118.30
1	B	582	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	92	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	571	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	B	374	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	106	ARG	NE-CZ-NH2	-5.84	117.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	360	CYS	CA-CB-SG	-5.79	103.58	114.00
1	A	510	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	B	460	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	B	576	ASP	CB-CG-OD1	-5.76	113.11	118.30
1	B	295	CYS	CA-CB-SG	-5.73	103.68	114.00
1	B	442	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	294	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	358	THR	OG1-CB-CG2	-5.53	97.28	110.00
1	A	285	ARG	CG-CD-NE	-5.51	100.22	111.80
1	A	555	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	103	PRO	N-CA-C	5.47	126.32	112.10
1	A	285	ARG	N-CA-CB	-5.47	100.75	110.60
1	B	351	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	285	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	385	ASP	CB-CG-OD1	-5.38	113.45	118.30
1	B	466	MET	CG-SD-CE	-5.38	91.59	100.20
1	A	139	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	535	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	347	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	596	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	413	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	B	54	THR	OG1-CB-CG2	-5.26	97.89	110.00
1	A	66	THR	OG1-CB-CG2	-5.20	98.04	110.00
1	B	546	LEU	CB-CG-CD2	5.20	119.83	111.00
1	A	522	ARG	CG-CD-NE	5.18	122.67	111.80
1	B	416[A]	SER	CB-CA-C	-5.17	100.28	110.10
1	B	416[B]	SER	CB-CA-C	-5.17	100.28	110.10
1	B	495	MET	CA-CB-CG	5.17	122.08	113.30
1	B	40	ARG	CB-CG-CD	5.16	125.02	111.60
1	A	431	LEU	CB-CG-CD1	5.15	119.75	111.00
1	A	293	PHE	CB-CG-CD1	5.14	124.40	120.80
1	A	208	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	189	ASP	OD1-CG-OD2	-5.09	113.62	123.30
1	B	229	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	535	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	264	MET	CG-SD-CE	-5.03	92.15	100.20
1	A	409	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	420	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	VAL	Peptide
1	A	229	ASP	Peptide
1	B	102	SER	Peptide
1	B	506	HIS	Sidechain

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	4508	0	4420	97	0
1	B	4717	0	4653	130	0
2	B	27	0	12	1	0
3	A	27	0	11	0	0
3	B	54	0	25	6	0
4	A	343	0	0	27	0
4	B	324	0	0	27	0
All	All	10000	0	9121	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (222) 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:553:ILE:CD1	1:B:553:ILE:CG1	1.75	1.63
1:B:466:MET:CE	1:B:466:MET:SD	2.04	1.46
1:A:466:MET:SD	1:A:466:MET:CE	2.04	1.44
1:A:70:MET:CE	1:A:70:MET:SD	2.07	1.41
1:B:329:MET:CE	1:B:329:MET:SD	2.08	1.41
1:B:578:GLU:O	1:B:579:HIS:CG	1.95	1.18
1:B:207:CYS:HB3	4:B:3118:HOH:O	1.52	1.08
1:B:489:ALA:CB	4:B:3119:HOH:O	2.06	1.04
1:A:367:LYS:HD3	4:A:3201:HOH:O	1.58	1.03
1:B:489:ALA:HB3	4:B:3119:HOH:O	1.61	1.00
1:B:578:GLU:O	1:B:579:HIS:ND1	1.94	0.99
1:B:92:ARG:NH1	1:B:100:GLY:O	1.96	0.97
1:A:346[B]:HIS:CD2	1:A:376:LEU:HD21	1.99	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLU:CD	1:A:241:GLU:H	1.66	0.96
1:A:578:GLU:O	1:A:579:HIS:CD2	2.19	0.94
1:A:370:MET:HG3	4:A:3230:HOH:O	1.66	0.94
1:A:235:LYS:HZ3	1:A:279:ASN:HD21	1.09	0.93
1:B:93:GLN:HG3	4:B:3121:HOH:O	1.69	0.93
1:A:596:ARG:HG3	4:A:3231:HOH:O	1.69	0.92
1:B:553:ILE:HG12	4:B:3123:HOH:O	1.71	0.90
1:A:235:LYS:NZ	1:A:279:ASN:HD21	1.73	0.86
1:B:180:GLY:O	1:B:181:GLU:HB3	1.75	0.85
3:B:2805:ADX:N3	3:B:2805:ADX:H2'	1.91	0.84
1:B:103:PRO:CA	4:B:3108:HOH:O	2.25	0.83
1:B:103:PRO:N	4:B:3108:HOH:O	2.11	0.83
1:B:579:HIS:HB3	1:B:582:ASP:OD1	1.78	0.82
1:B:578:GLU:O	1:B:579:HIS:CD2	2.33	0.81
1:B:392:GLY:O	1:B:395:GLN:NE2	2.11	0.81
1:A:346[B]:HIS:HD2	1:A:376:LEU:HD21	1.46	0.80
1:A:522:ARG:O	1:A:522:ARG:NH1	2.16	0.79
1:B:102:SER:C	4:B:3108:HOH:O	2.21	0.79
1:B:241:GLU:CD	1:B:241:GLU:H	1.86	0.78
1:B:578:GLU:O	1:B:579:HIS:CE1	2.37	0.77
1:B:103:PRO:HA	4:B:3108:HOH:O	1.83	0.77
1:A:452[B]:HIS:HD2	1:A:510:ARG:HE	1.30	0.76
1:B:241:GLU:N	1:B:241:GLU:CD	2.39	0.76
1:A:578:GLU:O	1:A:579:HIS:HD2	1.69	0.76
1:B:163:HIS:CE1	4:B:3129:HOH:O	2.38	0.76
1:B:96:ASN:HD21	1:B:112:ARG:HD2	1.49	0.75
1:A:346[B]:HIS:CE1	1:A:348:LYS:HG2	2.22	0.74
1:A:235:LYS:HZ3	1:A:279:ASN:ND2	1.86	0.73
1:A:235:LYS:NZ	1:A:279:ASN:ND2	2.37	0.72
1:A:283:ARG:HD2	4:A:3234:HOH:O	1.88	0.72
1:B:489:ALA:N	4:B:3119:HOH:O	2.23	0.72
1:B:163:HIS:HE1	4:B:3129:HOH:O	1.70	0.72
1:A:452[B]:HIS:CD2	1:A:510:ARG:HE	2.08	0.71
1:B:502:GLU:HG2	1:B:506:HIS:CE1	2.27	0.70
1:A:553:ILE:HD12	4:A:3137:HOH:O	1.92	0.70
1:B:93:GLN:CG	4:B:3121:HOH:O	2.31	0.70
1:B:186:THR:HB	4:B:3055:HOH:O	1.92	0.69
1:B:180:GLY:O	1:B:181:GLU:CB	2.39	0.69
1:A:161:PRO:C	4:A:3215:HOH:O	2.32	0.68
1:A:241:GLU:N	1:A:241:GLU:CD	2.42	0.68
1:B:420:LEU:HD13	1:B:453:PRO:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLY:HA2	1:B:189:ASP:HB2	1.76	0.67
1:A:79:HIS:CD2	4:A:3208:HOH:O	2.46	0.66
1:B:578:GLU:C	1:B:579:HIS:CG	2.69	0.66
1:B:579:HIS:O	1:B:581:GLU:N	2.29	0.65
1:B:245:HIS:HB2	4:B:3107:HOH:O	1.98	0.64
1:B:386:ARG:HG3	1:B:387:VAL:N	2.13	0.64
1:A:89:ASP:C	4:A:3209:HOH:O	2.36	0.63
1:A:452[B]:HIS:HE1	4:A:2922:HOH:O	1.82	0.62
1:B:545:VAL:HG21	1:A:292[A]:HIS:CD2	2.35	0.62
1:A:214:GLN:CG	4:A:3197:HOH:O	2.46	0.62
1:B:45:GLY:N	1:A:44:VAL:O	2.31	0.61
1:B:425:HIS:H	1:B:428:HIS:HD2	1.47	0.61
1:B:506:HIS:O	1:B:510:ARG:HD3	2.01	0.61
1:A:79:HIS:CG	4:A:3208:HOH:O	2.55	0.60
1:B:468:ARG:HD2	4:B:2817:HOH:O	2.00	0.60
1:A:47:ARG:HH11	1:A:227:PRO:HD2	1.67	0.59
1:A:405:GLN:NE2	1:A:409:ASP:OD2	2.34	0.59
1:B:607:ALA:HA	4:B:3116:HOH:O	2.01	0.59
1:A:371:GLU:HG3	4:A:3133:HOH:O	2.02	0.59
1:B:184:GLY:HA2	1:B:189:ASP:CB	2.32	0.59
1:B:196:GLU:HG3	4:B:3046:HOH:O	2.03	0.59
1:B:96:ASN:ND2	1:B:112:ARG:HD2	2.17	0.58
1:B:466:MET:CG	1:B:466:MET:CE	2.82	0.58
1:A:214:GLN:HG2	4:A:3197:HOH:O	2.04	0.58
1:A:75:TYR:C	1:A:75:TYR:CD1	2.77	0.57
1:A:596:ARG:CG	4:A:3231:HOH:O	2.41	0.57
1:A:370:MET:HE3	1:A:370:MET:HA	1.87	0.57
1:B:112:ARG:O	1:B:116:VAL:HG23	2.06	0.56
1:B:179:ALA:C	1:B:180:GLY:O	2.45	0.56
1:B:64:GLY:HA2	2:B:2800:ADP:H5'1	1.87	0.56
1:A:346[B]:HIS:ND1	1:A:348:LYS:CG	2.69	0.55
1:B:92:ARG:NH2	3:B:2805:ADX:O3B	2.40	0.54
1:B:346:HIS:HE1	1:B:351:ARG:HH11	1.55	0.54
1:A:231:SER:OG	1:A:404:LYS:HE2	2.08	0.54
1:B:40:ARG:HH11	1:B:40:ARG:CB	2.20	0.54
1:B:363:HIS:HB3	1:B:366:ILE:HB	1.90	0.54
1:A:239[B]:VAL:HG12	1:A:383:VAL:O	2.08	0.53
1:A:416[A]:SER:HB2	4:A:3233:HOH:O	2.09	0.53
1:B:420:LEU:HD13	1:B:453:PRO:CA	2.38	0.53
1:B:553:ILE:CG1	4:B:3123:HOH:O	2.44	0.53
1:B:524:PRO:O	1:B:525:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:HG2	1:B:174:TYR:CG	2.44	0.52
1:B:386:ARG:HG2	1:B:388:TYR:CE1	2.44	0.52
1:A:106:ARG:O	1:A:109:ASN:HB3	2.09	0.52
1:A:314:HIS:HD2	1:A:375:TRP:HE1	1.58	0.52
1:B:545:VAL:CG2	1:A:292[A]:HIS:HD2	2.22	0.52
1:A:340:ASN:N	1:A:341:PRO:HD3	2.25	0.52
1:A:529:HIS:CE1	1:A:531:GLU:HB2	2.45	0.51
1:B:341:PRO:HA	1:B:378:GLY:O	2.09	0.51
1:A:340:ASN:N	1:A:341:PRO:CD	2.73	0.51
1:B:106:ARG:HD2	3:B:2805:ADX:O1B	2.09	0.51
3:B:2805:ADX:C2'	3:B:2805:ADX:N3	2.71	0.51
1:B:340:ASN:N	1:B:341:PRO:HD3	2.26	0.51
1:A:416[B]:SER:HB3	4:A:3233:HOH:O	2.11	0.51
1:B:233:GLU:O	1:B:234:VAL:C	2.48	0.51
1:B:271:ALA:HB2	1:B:383:VAL:HG21	1.93	0.51
1:B:425:HIS:H	1:B:428:HIS:CD2	2.27	0.51
1:B:553:ILE:HG12	1:B:554:THR:N	2.25	0.50
1:A:317:LYS:HG2	1:A:343:PHE:CD2	2.46	0.50
1:A:214:GLN:HG3	4:A:3197:HOH:O	2.08	0.50
1:B:422:ASN:ND2	4:B:2905:HOH:O	2.43	0.50
1:B:601:PRO:HD3	1:B:611:TRP:CZ2	2.46	0.50
1:A:96:ASN:ND2	1:A:109:ASN:OD1	2.45	0.49
1:B:491:PHE:CE2	1:B:493:SER:HB3	2.47	0.49
1:A:363:HIS:HB3	1:A:366:ILE:HB	1.93	0.49
1:A:42:GLN:NE2	4:A:3185:HOH:O	2.44	0.49
1:B:450:LEU:HD21	1:B:452:HIS:ND1	2.26	0.49
1:B:215:GLN:O	4:B:2957:HOH:O	2.19	0.49
1:A:506:HIS:O	1:A:510:ARG:HD3	2.13	0.49
1:A:346[B]:HIS:HD1	1:A:348:LYS:CG	2.26	0.49
1:B:346:HIS:CE1	1:B:351:ARG:HH11	2.29	0.49
1:A:382:GLN:CD	4:A:3227:HOH:O	2.51	0.49
1:B:134:PRO:HD3	3:B:2805:ADX:O1B	2.13	0.49
1:B:425:HIS:CE1	1:B:428:HIS:NE2	2.81	0.49
1:A:370:MET:CG	4:A:3230:HOH:O	2.41	0.48
1:B:72:LEU:HD22	1:B:216:VAL:HG11	1.95	0.48
1:B:522:ARG:HG2	1:B:562:VAL:HB	1.96	0.48
1:B:292[B]:HIS:CE1	4:B:2834:HOH:O	2.66	0.48
1:B:618:TYR:O	1:B:622:GLU:HG2	2.14	0.48
1:B:149:ALA:O	1:B:150:SER:HB2	2.13	0.48
1:A:231:SER:OG	1:A:404:LYS:CE	2.62	0.47
1:A:79:HIS:CE1	4:A:3208:HOH:O	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LEU:HD23	1:B:481:LEU:O	2.14	0.47
1:A:420:LEU:HD13	1:A:453:PRO:HA	1.96	0.47
1:A:579:HIS:O	1:A:580:HIS:C	2.52	0.47
1:A:316:ASP:HB2	4:A:3077:HOH:O	2.14	0.47
1:A:346[B]:HIS:ND1	1:A:348:LYS:HG2	2.30	0.47
1:B:108:GLU:OE1	1:B:108:GLU:HA	2.13	0.47
1:B:622:GLU:O	1:B:623:LYS:HG3	2.14	0.47
1:B:101:PHE:HB2	1:B:183:LYS:HD3	1.95	0.47
1:A:356:TRP:CD1	1:A:498:ALA:HB2	2.50	0.47
1:B:40:ARG:HH11	1:B:40:ARG:CG	2.27	0.47
1:B:565:TYR:CZ	1:B:602:PRO:HB2	2.51	0.46
1:B:174:TYR:HD2	1:B:188:ILE:HD11	1.80	0.46
1:A:466:MET:CG	1:A:466:MET:CE	2.91	0.46
1:B:235:LYS:NZ	1:B:279:ASN:OD1	2.40	0.46
1:B:186:THR:HG23	3:B:2805:ADX:H2	1.97	0.46
1:B:579:HIS:O	1:B:580:HIS:C	2.53	0.46
1:B:579:HIS:C	1:B:581:GLU:N	2.67	0.46
1:A:452[B]:HIS:HD2	1:A:510:ARG:NE	2.05	0.46
1:B:446:ARG:N	1:B:447:PRO:CD	2.78	0.46
1:B:166:GLU:HG2	1:B:174:TYR:CD2	2.50	0.46
1:A:243:LYS:NZ	4:A:3186:HOH:O	2.48	0.45
1:B:292[B]:HIS:HE1	4:B:2834:HOH:O	1.99	0.45
1:A:83:CYS:HA	1:A:126:VAL:O	2.17	0.45
1:B:101:PHE:CD1	1:B:101:PHE:N	2.84	0.45
1:B:395:GLN:HG3	4:B:3089:HOH:O	2.16	0.45
1:A:346[A]:HIS:CE1	1:A:351:ARG:HH11	2.35	0.45
1:B:507:CYS:HA	1:B:518:TYR:CE1	2.52	0.45
1:A:239[B]:VAL:HG23	1:A:240:PRO:HD2	1.99	0.44
1:A:81:ILE:HD13	1:A:226:VAL:HG22	1.98	0.44
1:A:330:TYR:OH	4:A:3190:HOH:O	2.21	0.44
1:B:123:ALA:HB2	1:A:84:TYR:CD1	2.52	0.44
1:B:40:ARG:CG	1:B:40:ARG:NH1	2.78	0.44
1:A:108:GLU:O	1:A:112:ARG:HG3	2.17	0.44
1:A:386:ARG:HE	1:A:386:ARG:HB3	1.50	0.44
1:A:346[B]:HIS:HE1	1:A:369:VAL:HG13	1.83	0.44
1:B:57:LEU:HD23	1:B:156:VAL:HB	1.99	0.44
1:B:520:VAL:O	1:B:559:PRO:HA	2.18	0.44
1:A:408:LYS:O	1:A:411:ASN:N	2.42	0.43
1:B:361:LYS:HE3	4:B:3090:HOH:O	2.18	0.43
1:A:271:ALA:HB2	1:A:383:VAL:HG21	2.00	0.43
1:B:188:ILE:HG22	1:B:189:ASP:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:VAL:HG13	1:B:575:TYR:HB3	2.01	0.43
1:B:539:PRO:HB3	4:B:3115:HOH:O	2.18	0.43
1:B:96:ASN:ND2	1:B:112:ARG:HH11	2.17	0.42
1:A:231:SER:OG	1:A:404:LYS:NZ	2.51	0.42
1:B:184:GLY:O	1:B:190:SER:OG	2.19	0.42
1:A:392:GLY:O	1:A:395:GLN:NE2	2.43	0.42
1:A:452[A]:HIS:ND1	1:A:510:ARG:NE	2.60	0.42
1:A:70:MET:CE	1:A:70:MET:CG	2.95	0.42
1:B:543:ALA:O	1:B:547:THR:HG23	2.20	0.42
1:B:606:MET:SD	1:B:614:LEU:HD12	2.60	0.42
1:A:497:TYR:N	1:A:502:GLU:OE1	2.52	0.42
1:A:561:ARG:NE	4:A:3122:HOH:O	2.47	0.42
1:B:386:ARG:HG3	1:B:387:VAL:H	1.83	0.42
1:A:341:PRO:HA	1:A:378:GLY:O	2.20	0.42
1:A:452[B]:HIS:CD2	1:A:510:ARG:NE	2.83	0.42
1:B:40:ARG:CB	1:B:40:ARG:NH1	2.83	0.41
1:B:523:ASP:N	1:B:524:PRO:CD	2.83	0.41
1:A:511:MET:HB2	1:A:555:LEU:HD13	2.03	0.41
1:B:85:THR:HB	1:A:34:HIS:HE1	1.85	0.41
1:A:196:GLU:CG	4:A:3212:HOH:O	2.68	0.41
1:B:239:VAL:HG23	1:B:240:PRO:HD2	2.01	0.41
1:B:596:ARG:C	1:B:598:GLY:H	2.24	0.41
1:B:82:PRO:HG3	1:A:44:VAL:HA	2.02	0.41
1:B:172:GLY:O	1:B:176:LYS:HB2	2.20	0.41
1:B:247:ALA:O	1:B:251:ALA:N	2.48	0.41
1:B:440:LEU:HD23	1:B:440:LEU:HA	1.89	0.41
1:B:558:VAL:HG12	1:B:560:PHE:CE1	2.55	0.41
1:B:66:THR:O	1:B:70:MET:HG2	2.20	0.41
1:B:549:ALA:HA	1:B:550:PRO:HD3	1.86	0.41
1:A:435:THR:O	1:A:439:LEU:HG	2.20	0.41
1:B:261:LYS:O	1:B:265:GLN:HG3	2.21	0.41
1:B:278:LEU:HA	1:B:278:LEU:HD23	1.87	0.41
1:A:134:PRO:HA	1:A:192:TYR:CD2	2.56	0.41
1:A:248:LYS:HE3	4:A:3243:HOH:O	2.20	0.41
1:B:545:VAL:CG2	1:A:292[A]:HIS:CD2	2.99	0.41
1:B:51:ARG:NE	1:B:225:ILE:O	2.50	0.41
1:A:360:CYS:SG	1:A:530:PRO:HG2	2.60	0.41
1:B:465:LEU:O	1:B:466:MET:C	2.59	0.41
1:B:398:LEU:N	1:B:398:LEU:CD1	2.83	0.40
1:B:314:HIS:CE1	1:B:375:TRP:HE1	2.39	0.40
1:A:621:LEU:HD23	1:A:621:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ARG:NH1	4:B:3113:HOH:O	2.54	0.40
1:B:440:LEU:HD23	1:B:444:TYR:O	2.22	0.40
1:A:596:ARG:HB3	1:A:596:ARG:HH11	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/630 (90%)	547 (97%)	17 (3%)	2 (0%)	34	22
1	B	591/630 (94%)	557 (94%)	24 (4%)	10 (2%)	9	2
All	All	1157/1260 (92%)	1104 (95%)	41 (4%)	12 (1%)	15	6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	SER
1	B	103	PRO
1	B	183	LYS
1	B	579	HIS
1	A	230	ALA
1	B	580	HIS
1	A	579	HIS
1	B	169	ASP
1	B	180	GLY
1	B	181	GLU
1	B	568	LYS
1	B	332	GLY

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	489/538 (91%)	452 (92%)	37 (8%)	13	4
1	B	507/538 (94%)	463 (91%)	44 (9%)	10	2
All	All	996/1076 (93%)	915 (92%)	81 (8%)	12	3

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	34	HIS
1	B	38	ASN
1	B	40	ARG
1	B	92	ARG
1	B	102	SER
1	B	106	ARG
1	B	130	SER
1	B	144	GLN
1	B	162	LEU
1	B	163	HIS
1	B	167	GLN
1	B	171	LYS
1	B	173	LEU
1	B	176	LYS
1	B	182	ILE
1	B	186	THR
1	B	241	GLU
1	B	243	LYS
1	B	246	LEU
1	B	304	LEU
1	B	310[A]	LEU
1	B	310[B]	LEU
1	B	314	HIS
1	B	323	CYS
1	B	419	GLN
1	B	420	LEU
1	B	437	LYS

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Mol	Chain	Res	Type
1	B	508	ARG
1	B	522	ARG
1	B	531	GLU
1	B	553	ILE
1	B	555	LEU
1	B	567	LYS
1	B	570	LYS
1	B	571	ARG
1	B	577	SER
1	B	581	GLU
1	B	589	THR
1	B	593	LYS
1	B	609	LYS
1	B	616	GLU
1	B	619	LYS
1	B	621	LEU
1	B	622	GLU
1	A	39	LYS
1	A	40	ARG
1	A	42	GLN
1	A	46	THR
1	A	70	MET
1	A	82	PRO
1	A	93	GLN
1	A	150	SER
1	A	196	GLU
1	A	206	SER
1	A	207	CYS
1	A	214	GLN
1	A	222	GLU
1	A	241	GLU
1	A	246	LEU
1	A	304	LEU
1	A	346[A]	HIS
1	A	346[B]	HIS
1	A	347	ARG
1	A	386	ARG
1	A	420	LEU
1	A	445	ARG
1	A	508	ARG
1	A	522	ARG
1	A	534	LYS

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Mol	Chain	Res	Type
1	A	553	ILE
1	A	555	LEU
1	A	568	LYS
1	A	570	LYS
1	A	571	ARG
1	A	577	SER
1	A	578	GLU
1	A	581	GLU
1	A	582	ASP
1	A	596	ARG
1	A	597	GLU
1	A	609	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	ASN
1	B	109	ASN
1	B	163	HIS
1	B	210	ASN
1	B	346	HIS
1	B	422	ASN
1	B	425	HIS
1	B	436	HIS
1	B	599	GLN
1	A	140	ASN
1	A	279	ASN
1	A	314	HIS
1	A	422	ASN
1	A	579	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ADX	B	2805	-	25,29,29	1.68	4 (16%)	26,45,45	2.78	12 (46%)
2	ADP	B	2800	-	24,29,29	1.69	3 (12%)	29,45,45	1.60	4 (13%)
3	ADX	B	2700	-	25,29,29	2.11	10 (40%)	26,45,45	2.87	9 (34%)
3	ADX	A	2900	-	25,29,29	2.23	8 (32%)	26,45,45	2.40	8 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADX	B	2805	-	-	1/6/32/32	0/3/3/3
2	ADP	B	2800	-	-	2/12/32/32	0/3/3/3
3	ADX	B	2700	-	-	2/6/32/32	0/3/3/3
3	ADX	A	2900	-	-	2/6/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2900	ADX	PA-O3A	5.12	1.63	1.59
3	A	2900	ADX	O4'-C1'	4.78	1.47	1.41
2	B	2800	ADP	C2-N3	4.40	1.39	1.32
3	B	2700	ADX	PA-O3A	4.08	1.62	1.59
3	A	2900	ADX	C2'-C1'	-3.88	1.47	1.53
3	B	2805	ADX	C2-N3	3.83	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2700	ADX	C2-N1	3.83	1.41	1.33
3	A	2900	ADX	C2-N3	3.59	1.37	1.32
3	B	2805	ADX	PA-O3A	3.53	1.62	1.59
3	A	2900	ADX	O2'-C2'	-3.41	1.35	1.43
3	B	2700	ADX	PA-O1A	-3.38	1.38	1.50
2	B	2800	ADP	C2'-C1'	-3.29	1.48	1.53
3	B	2805	ADX	O2B-SB	3.29	1.59	1.45
3	B	2700	ADX	C2'-C1'	3.07	1.58	1.53
3	B	2805	ADX	C2-N1	3.05	1.39	1.33
3	A	2900	ADX	C8-N7	3.00	1.40	1.34
2	B	2800	ADP	C8-N7	3.00	1.40	1.34
3	B	2700	ADX	C8-N7	2.83	1.39	1.34
3	A	2900	ADX	C4-N3	-2.76	1.31	1.35
3	B	2700	ADX	O4'-C1'	2.71	1.44	1.41
3	B	2700	ADX	C3'-C4'	2.64	1.59	1.53
3	B	2700	ADX	PA-O5'	-2.45	1.49	1.59
3	A	2900	ADX	PA-O5'	-2.43	1.49	1.59
3	B	2700	ADX	C6-C5	-2.20	1.35	1.43
3	B	2700	ADX	C2-N3	2.14	1.35	1.32

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2700	ADX	O3B-SB-O2B	8.78	139.01	108.49
3	B	2805	ADX	N3-C2-N1	-7.71	116.63	128.68
3	A	2900	ADX	N3-C2-N1	-7.15	117.50	128.68
3	B	2700	ADX	O3A-PA-O5'	6.91	123.15	102.98
3	B	2805	ADX	C3'-C2'-C1'	5.26	108.90	100.98
3	B	2805	ADX	C5-C6-N6	-5.03	112.71	120.35
3	B	2700	ADX	N3-C2-N1	-4.93	120.97	128.68
2	B	2800	ADP	N3-C2-N1	-4.82	121.14	128.68
3	A	2900	ADX	O4'-C1'-C2'	-4.19	100.80	106.93
3	B	2805	ADX	O4'-C1'-C2'	-4.13	100.89	106.93
3	A	2900	ADX	C2-N1-C6	3.97	125.55	118.75
3	B	2805	ADX	O2B-SB-O1B	-3.63	97.66	112.22
3	B	2700	ADX	O2'-C2'-C3'	3.58	123.40	111.82
3	A	2900	ADX	O3B-SB-O2B	3.54	120.81	108.49
3	A	2900	ADX	C5-C6-N6	3.27	125.33	120.35
2	B	2800	ADP	O2A-PA-O5'	3.24	122.78	107.75
3	B	2805	ADX	N6-C6-N1	2.84	124.47	118.57
3	B	2805	ADX	O3B-SB-O2B	2.79	118.20	108.49
2	B	2800	ADP	O2A-PA-O1A	-2.74	98.71	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2805	ADX	O2A-PA-O5'	2.69	120.25	107.75
3	B	2700	ADX	O2'-C2'-C1'	-2.69	100.92	110.85
3	B	2805	ADX	O3'-C3'-C4'	2.65	118.72	111.05
3	A	2900	ADX	O2B-SB-O1B	-2.53	102.08	112.22
3	A	2900	ADX	C1'-N9-C4	-2.52	122.22	126.64
3	B	2700	ADX	O5'-C5'-C4'	2.48	117.51	108.99
3	B	2700	ADX	C5-C6-N6	-2.42	116.68	120.35
3	B	2700	ADX	O3'-C3'-C2'	-2.30	104.37	111.82
3	B	2805	ADX	C1'-N9-C4	-2.28	122.63	126.64
2	B	2800	ADP	O2B-PB-O3A	2.24	112.14	104.64
3	B	2805	ADX	O3A-PA-O5'	-2.14	96.72	102.98
3	B	2805	ADX	O4'-C4'-C3'	2.06	109.20	105.11
3	B	2700	ADX	C5-C6-N1	-2.06	115.67	120.35
3	A	2900	ADX	O4'-C4'-C5'	2.02	116.02	109.37

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2805	ADX	C5'-O5'-PA-O1A
3	A	2900	ADX	C5'-O5'-PA-O1A
3	A	2900	ADX	C5'-O5'-PA-O3A
2	B	2800	ADP	PA-O3A-PB-O1B
3	B	2700	ADX	C3'-C4'-C5'-O5'
2	B	2800	ADP	O4'-C4'-C5'-O5'
3	B	2700	ADX	O4'-C4'-C5'-O5'

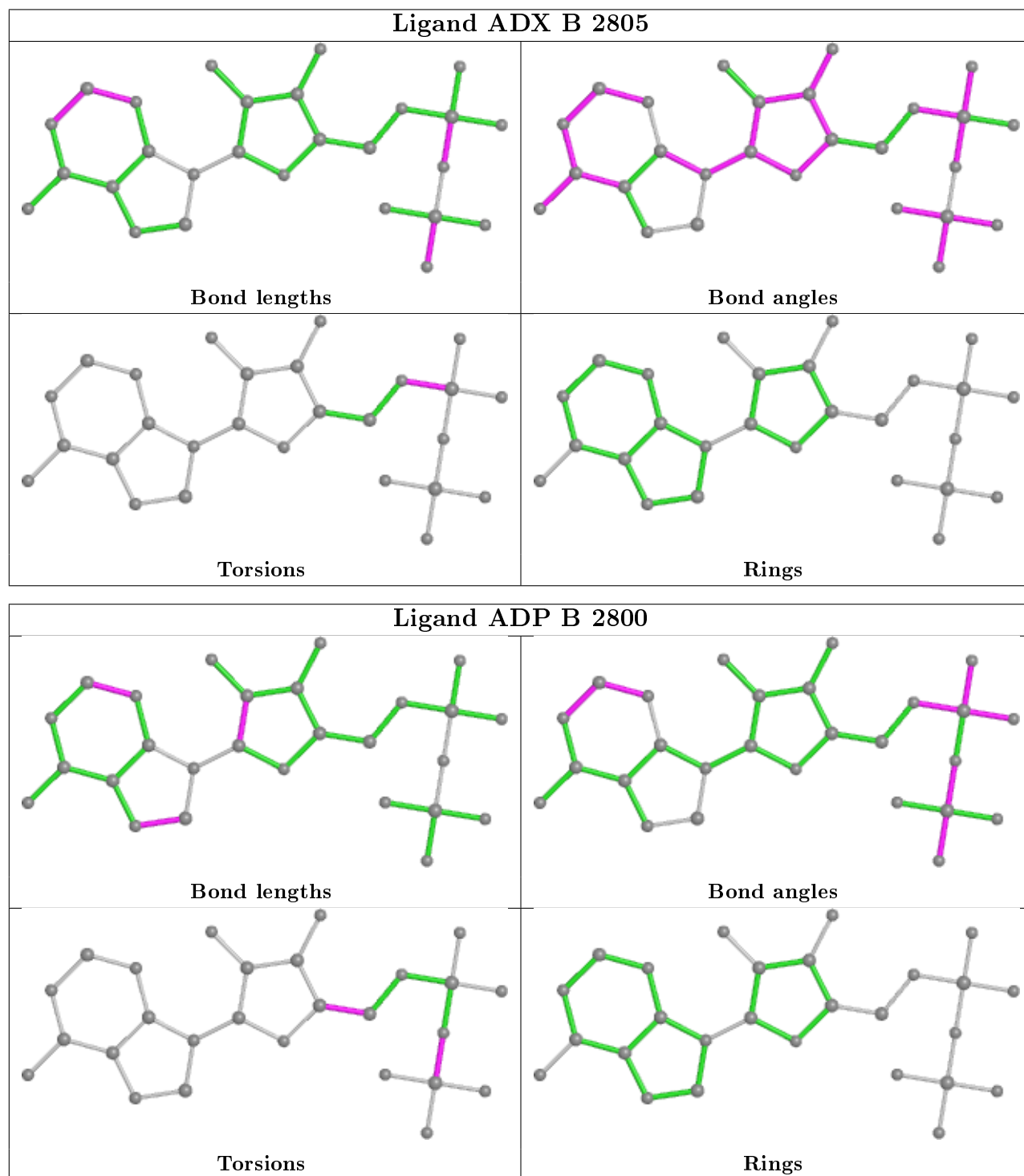
There are no ring outliers.

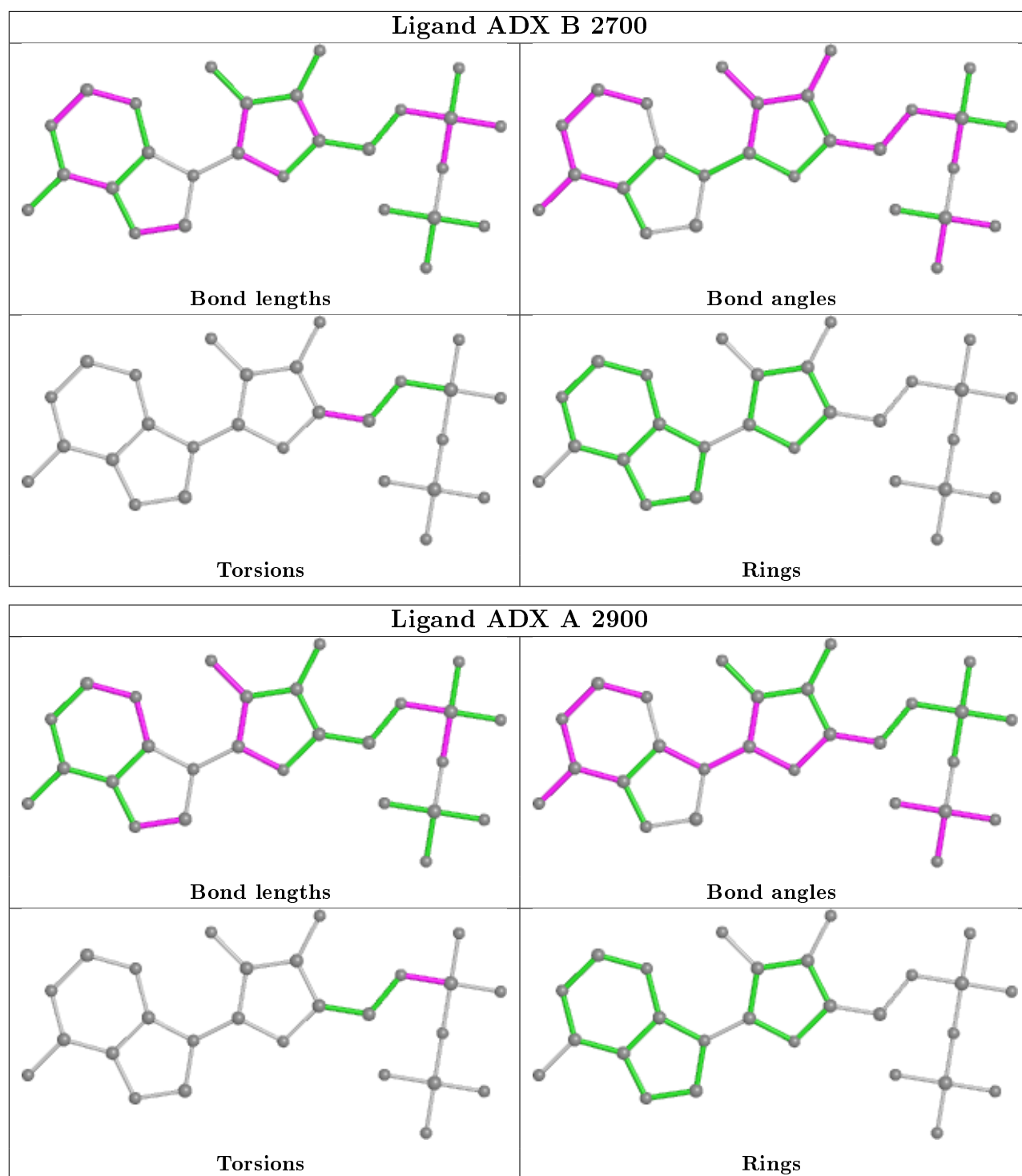
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2805	ADX	6	0
2	B	2800	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	562/630 (89%)	0.34	38 (6%)	17 19	17, 34, 60, 82	2 (0%)
1	B	590/630 (93%)	0.32	49 (8%)	11 12	19, 36, 65, 88	0
All	All	1152/1260 (91%)	0.33	87 (7%)	13 15	17, 35, 63, 88	2 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	ALA	5.9
1	B	181	GLU	4.9
1	B	175	LYS	4.2
1	B	595	ALA	4.2
1	B	596	ARG	4.0
1	B	621	LEU	3.9
1	B	182	ILE	3.8
1	A	577	SER	3.7
1	A	578	GLU	3.7
1	A	207	CYS	3.5
1	B	189	ASP	3.4
1	B	593	LYS	3.4
1	B	623	LYS	3.4
1	B	178	ARG	3.3
1	B	603	GLU	3.3
1	A	206	SER	3.3
1	B	598	GLY	3.2
1	B	174	TYR	3.2
1	B	318	GLU	3.1
1	A	205	ASP	3.1
1	A	624	ALA	3.1
1	A	229	ASP	3.1
1	A	232	TYR	3.1
1	B	420	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	321	ASP	3.0
1	A	161	PRO	3.0
1	B	197	ALA	3.0
1	B	597	GLU	2.9
1	A	306	VAL	2.9
1	B	565	TYR	2.8
1	A	86	LEU	2.8
1	B	599	GLN	2.8
1	A	116	VAL	2.8
1	B	144	GLN	2.8
1	B	315	GLU	2.8
1	A	503	VAL	2.8
1	B	180	GLY	2.7
1	A	498	ALA	2.6
1	B	577	SER	2.6
1	B	454	LEU	2.6
1	B	570	LYS	2.6
1	B	149	ALA	2.6
1	A	48	GLY	2.6
1	A	568	LYS	2.5
1	B	611	TRP	2.5
1	A	323[A]	CYS	2.5
1	B	618	TYR	2.5
1	B	176	LYS	2.5
1	A	505	TRP	2.5
1	B	190	SER	2.5
1	B	585	PHE	2.5
1	B	173	LEU	2.5
1	B	314	HIS	2.5
1	A	507	CYS	2.4
1	A	46	THR	2.4
1	A	454	LEU	2.4
1	B	622	GLU	2.4
1	A	417	ALA	2.4
1	A	38	ASN	2.4
1	A	518	TYR	2.3
1	B	601	PRO	2.3
1	A	304	LEU	2.3
1	B	580	HIS	2.2
1	B	185	PHE	2.2
1	B	490	ILE	2.2
1	B	291	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	594	LEU	2.2
1	B	267	VAL	2.2
1	A	509	ALA	2.2
1	A	581	GLU	2.2
1	A	491	PHE	2.2
1	A	128	ILE	2.1
1	A	314	HIS	2.1
1	B	163	HIS	2.1
1	A	290[A]	CYS	2.1
1	A	274	TRP	2.1
1	B	494	PRO	2.1
1	B	503	VAL	2.1
1	A	209	VAL	2.1
1	B	495	MET	2.0
1	A	113	ILE	2.0
1	B	578	GLU	2.0
1	A	230	ALA	2.0
1	A	494	PRO	2.0
1	B	505	TRP	2.0
1	A	576	ASP	2.0
1	B	581	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADX	B	2805	27/27	0.95	0.15	49,61,71,73	0
2	ADP	B	2800	27/27	0.97	0.09	40,46,48,52	0

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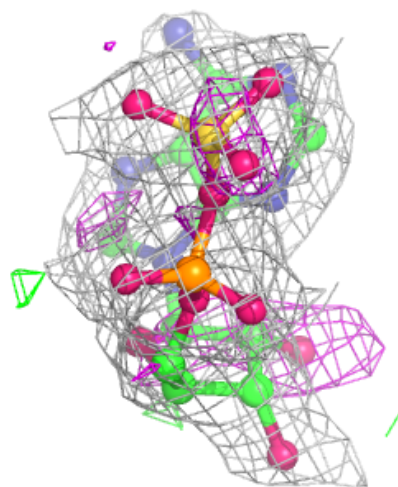
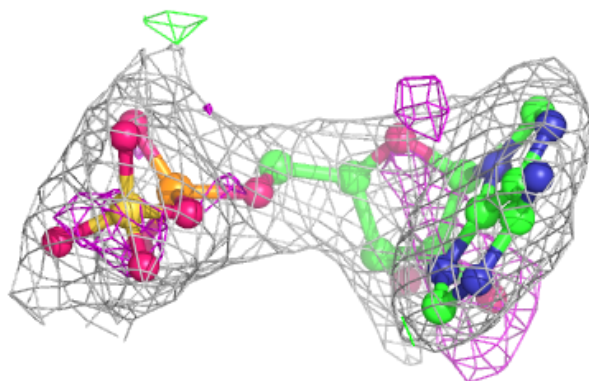
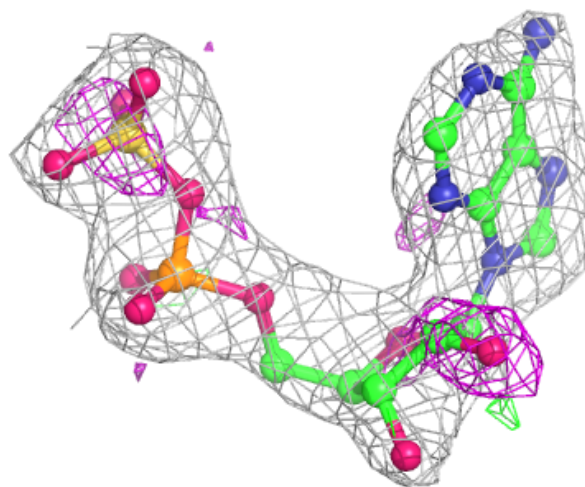
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADX	B	2700	27/27	0.98	0.12	28,34,41,42	0
3	ADX	A	2900	27/27	0.99	0.11	24,30,33,34	0

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.

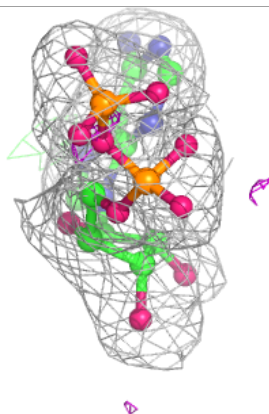
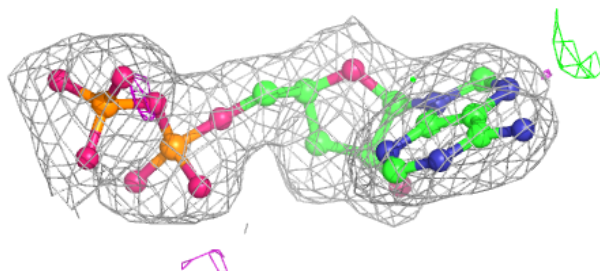
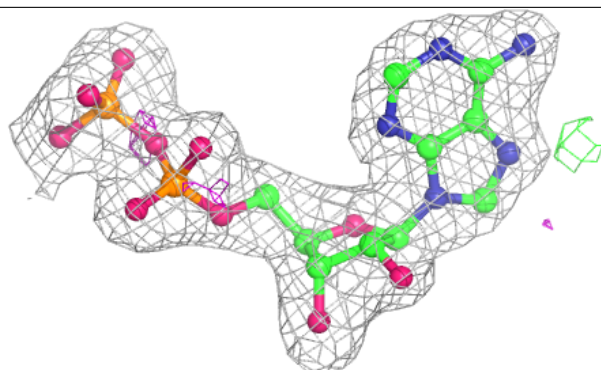
Electron density around ADX B 2805:

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

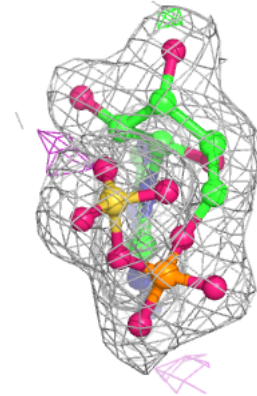
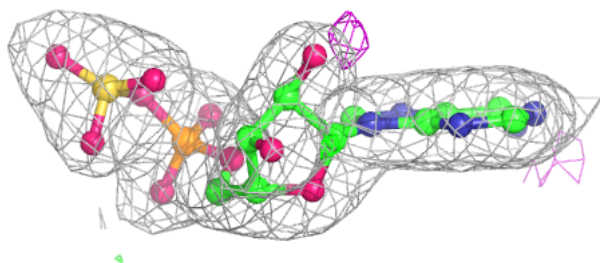
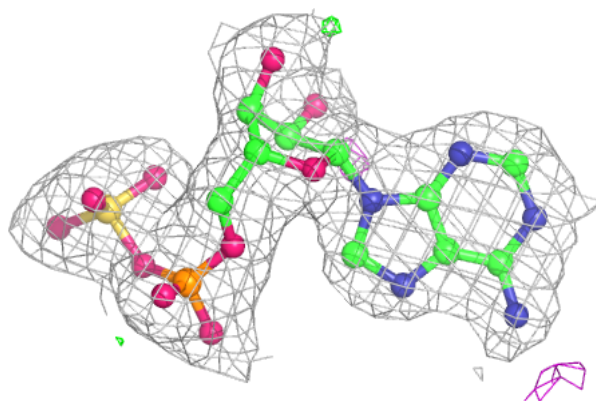


Electron density around ADP B 2800:

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

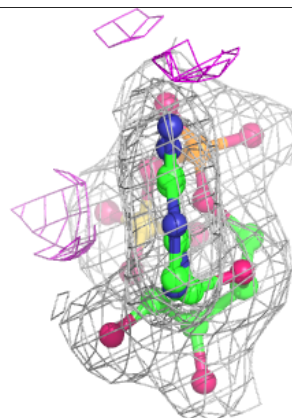
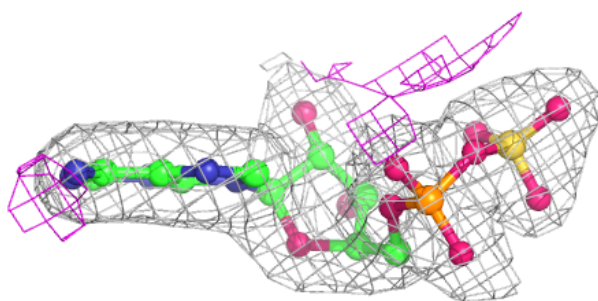
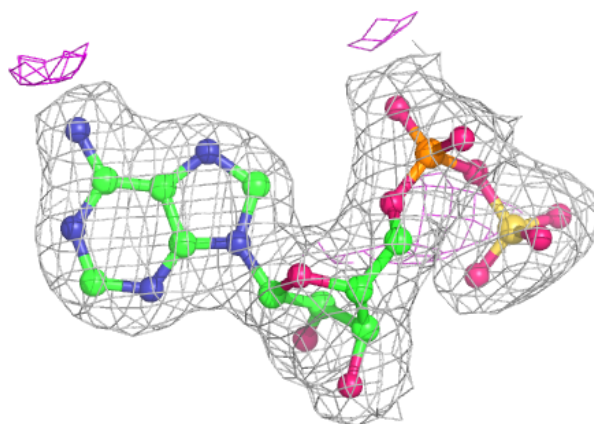
**Electron density around ADX B 2700:**

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



Electron density around ADX A 2900:

$2mF_o-DF_c$ (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.