



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:44 AM UTC

PDB ID : 1XNJ / pdb_00001xnj
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

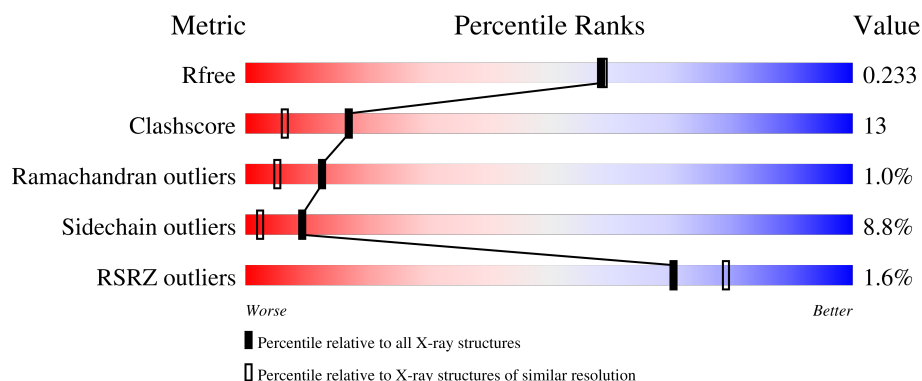
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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

Mol	Chain	Length	Quality of chain
1	A	630	2% 56% 26% 6% • 11%
1	B	630	% 50% 33% 9% • 6%

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.

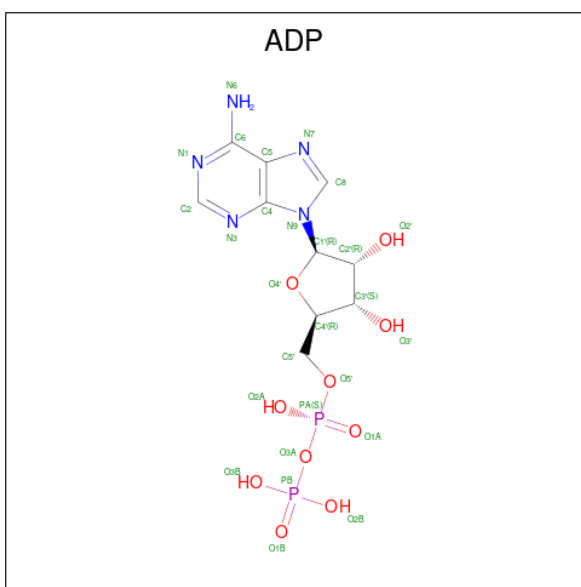
- Molecule 1 is a protein called Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1.

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:

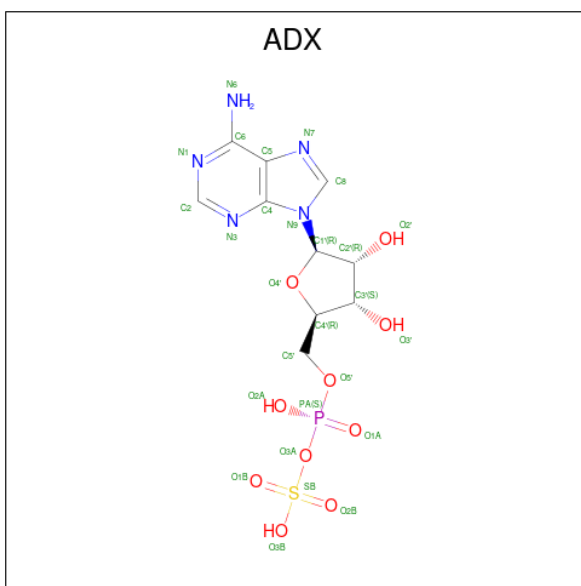
Chain	Residue	Modelled	Actual	Comment	Reference
B	416	SER	PHE	conflict	UNP O43252
B	625	HIS	-	expression tag	UNP O43252
B	626	HIS	-	expression tag	UNP O43252
B	627	HIS	-	expression tag	UNP O43252
B	628	HIS	-	expression tag	UNP O43252
B	629	HIS	-	expression tag	UNP O43252
B	630	HIS	-	expression tag	UNP 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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is ADENOSINE-5'-PHOSPHOSULFATE (CCD ID: ADX) (formula: $C_{10}H_{14}N_5O_{10}PS$).



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

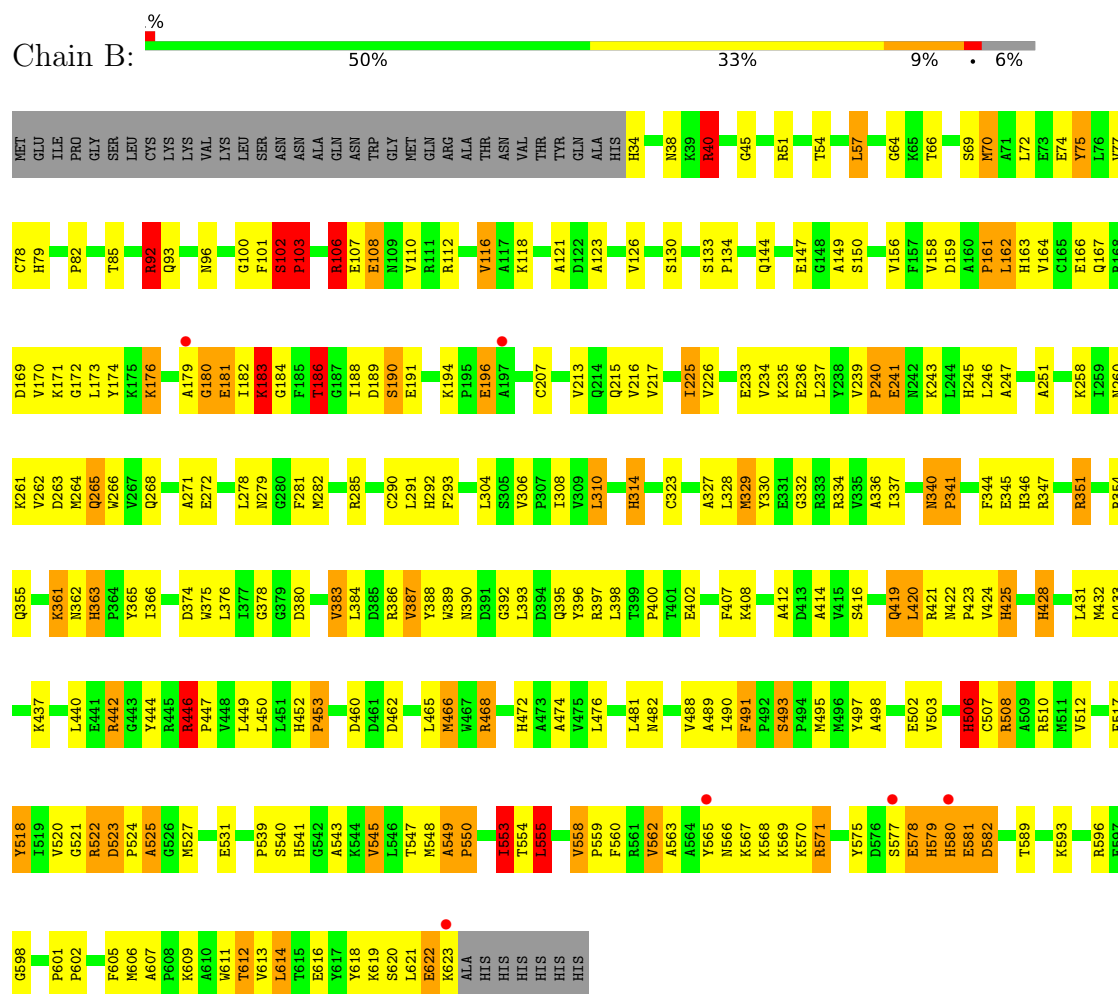
- Molecule 4 is water.

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

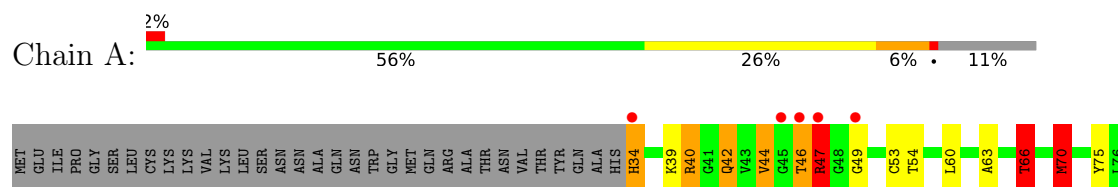
3 Residue-property plots

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: 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 – 1.98 128.47 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.0 (129.10-1.98) 97.6 (128.47-1.98)	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 (Not available) , 0.233	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 , 45.5	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	1.99	101/4663 (2.2%)	1.57	48/6321 (0.8%)
1	B	2.08	138/4846 (2.8%)	1.64	52/6563 (0.8%)
All	All	2.04	239/9509 (2.5%)	1.60	100/12884 (0.8%)

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 (239) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	ASN	CA-C	-14.25	1.44	1.53
1	B	329	MET	SD-CE	11.66	2.08	1.79
1	A	70	MET	SD-CE	11.08	2.07	1.79
1	B	491	PHE	CA-C	-10.93	1.41	1.52
1	B	433	GLN	CA-C	-10.04	1.39	1.52
1	A	466	MET	SD-CE	9.96	2.04	1.79
1	B	262	VAL	C-O	-9.82	1.12	1.24
1	A	348	LYS	CA-C	-9.81	1.39	1.52
1	B	466	MET	SD-CE	9.77	2.04	1.79
1	A	234	VAL	C-O	-9.48	1.13	1.24
1	B	340	ASN	C-O	-9.47	1.19	1.23
1	B	548	MET	SD-CE	-9.46	1.55	1.79
1	A	524	PRO	C-O	-9.14	1.13	1.23
1	B	121	ALA	CA-CB	-8.81	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	592	ARG	NE-CZ	8.68	1.42	1.33
1	A	334	ARG	C-O	-8.33	1.13	1.24
1	A	111	ARG	NE-CZ	-8.31	1.24	1.33
1	B	453	PRO	CA-CB	8.19	1.64	1.53
1	A	63	ALA	C-O	-8.05	1.14	1.24
1	B	236	GLU	CA-C	-7.98	1.42	1.52
1	B	497	TYR	CA-C	7.98	1.63	1.53
1	A	244	LEU	C-O	7.92	1.33	1.24
1	B	421	ARG	CA-C	7.90	1.62	1.52
1	B	416[A]	SER	CA-C	-7.79	1.43	1.52
1	B	416[B]	SER	CA-C	-7.79	1.43	1.52
1	B	614	LEU	C-O	7.78	1.33	1.24
1	B	110	VAL	CA-CB	-7.68	1.45	1.54
1	B	540	SER	N-CA	-7.65	1.35	1.46
1	A	267	VAL	CA-CB	-7.64	1.45	1.54
1	A	114	ALA	CA-CB	-7.62	1.41	1.53
1	A	271	ALA	CA-CB	-7.58	1.41	1.53
1	B	495	MET	SD-CE	-7.49	1.60	1.79
1	A	226	VAL	CA-C	7.46	1.59	1.53
1	B	460	ASP	C-O	-7.46	1.15	1.24
1	B	490	ILE	CA-CB	-7.46	1.45	1.54
1	B	268	GLN	CA-C	-7.44	1.43	1.52
1	B	70	MET	SD-CE	7.41	1.98	1.79
1	B	376	LEU	CA-C	-7.39	1.43	1.52
1	A	471	GLN	CA-C	-7.38	1.43	1.52
1	B	330	TYR	CA-C	7.31	1.61	1.52
1	A	501	THR	CA-CB	-7.27	1.41	1.53
1	A	268	GLN	CA-C	-7.22	1.43	1.52
1	A	120	PHE	N-CA	7.21	1.55	1.46
1	A	368	MET	CG-SD	7.20	1.98	1.80
1	B	553	ILE	CA-CB	7.18	1.64	1.54
1	B	545	VAL	CA-CB	-7.18	1.45	1.54
1	B	424	VAL	CA-CB	-7.17	1.45	1.54
1	B	158	VAL	CA-CB	-7.16	1.46	1.53
1	B	428	HIS	CA-CB	-7.14	1.42	1.53
1	B	512	VAL	N-CA	-7.14	1.37	1.46
1	B	306	VAL	N-CA	-7.13	1.37	1.46
1	B	488	VAL	CA-CB	7.13	1.62	1.54
1	B	121	ALA	CA-C	7.09	1.62	1.52
1	B	308	ILE	CA-C	-7.01	1.43	1.52
1	B	518	TYR	C-O	-6.97	1.16	1.24
1	B	77	VAL	CA-CB	-6.97	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	400	PRO	C-O	-6.93	1.15	1.24
1	B	108	GLU	CA-C	6.92	1.61	1.52
1	B	327	ALA	CA-C	-6.90	1.44	1.52
1	A	271	ALA	CA-C	-6.89	1.43	1.52
1	B	389	TRP	CA-C	6.85	1.61	1.52
1	A	509	ALA	CA-CB	-6.81	1.42	1.53
1	B	190	SER	N-CA	6.79	1.53	1.45
1	B	116	VAL	CA-CB	-6.78	1.46	1.54
1	A	231	SER	CA-C	6.70	1.61	1.52
1	A	454	LEU	CA-CB	6.68	1.64	1.53
1	A	46	THR	CA-CB	6.66	1.65	1.53
1	B	186	THR	CA-CB	6.63	1.64	1.53
1	A	511	MET	CA-C	-6.61	1.44	1.52
1	B	449	LEU	CA-C	-6.56	1.44	1.52
1	B	293	PHE	C-O	-6.55	1.15	1.24
1	B	558	VAL	CA-C	6.54	1.59	1.52
1	B	336	ALA	CA-C	-6.51	1.44	1.52
1	A	514	GLY	C-O	-6.50	1.15	1.24
1	A	476	LEU	CA-C	6.45	1.61	1.52
1	A	586	ILE	CA-CB	-6.43	1.46	1.53
1	B	265	GLN	CA-C	6.41	1.61	1.52
1	A	128	ILE	CA-CB	6.40	1.61	1.54
1	B	562	VAL	C-O	-6.38	1.17	1.24
1	B	380	ASP	C-O	-6.37	1.16	1.24
1	B	266	TRP	N-CA	6.34	1.54	1.46
1	B	503	VAL	N-CA	-6.34	1.39	1.46
1	A	464	PRO	CA-C	-6.32	1.45	1.52
1	A	95	LEU	N-CA	-6.31	1.38	1.46
1	B	310[A]	LEU	C-O	6.31	1.31	1.24
1	B	310[B]	LEU	C-O	6.31	1.31	1.24
1	B	419	GLN	CG-CD	-6.29	1.36	1.52
1	B	506	HIS	CG-ND1	-6.28	1.31	1.38
1	B	170	VAL	CA-CB	6.25	1.64	1.54
1	B	282	MET	SD-CE	-6.24	1.64	1.79
1	B	74	GLU	C-O	-6.24	1.17	1.24
1	A	414	ALA	CA-CB	-6.22	1.43	1.53
1	A	302	ILE	CA-C	-6.21	1.44	1.52
1	A	489	ALA	C-O	-6.16	1.16	1.23
1	B	396	TYR	CA-C	6.16	1.61	1.52
1	B	40	ARG	CB-CG	6.14	1.70	1.52
1	B	337	ILE	CA-C	6.14	1.60	1.52
1	B	488	VAL	N-CA	-6.13	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	TYR	C-O	-6.13	1.16	1.24
1	B	517	PHE	C-O	-6.11	1.16	1.23
1	B	285	ARG	NE-CZ	-6.11	1.26	1.33
1	A	337	ILE	CA-CB	6.08	1.61	1.54
1	B	126	VAL	C-O	6.08	1.30	1.24
1	B	260	ASN	CA-C	-6.08	1.44	1.53
1	A	44	VAL	C-O	6.04	1.30	1.24
1	A	353	ALA	C-O	6.04	1.31	1.24
1	B	553	ILE	CG1-CD1	6.03	1.75	1.51
1	B	449	LEU	C-O	6.02	1.31	1.24
1	B	347	ARG	CZ-NH1	6.00	1.41	1.32
1	B	191	GLU	C-O	6.00	1.31	1.23
1	A	308	ILE	CA-CB	-5.99	1.46	1.53
1	B	462	ASP	CA-C	5.99	1.61	1.53
1	A	518	TYR	CZ-OH	-5.95	1.25	1.38
1	B	345	GLU	CD-OE1	5.95	1.36	1.25
1	B	362	ASN	C-O	-5.95	1.16	1.24
1	B	549	ALA	CA-C	-5.95	1.46	1.53
1	B	563	ALA	C-O	-5.94	1.16	1.23
1	B	402	GLU	C-O	-5.93	1.17	1.24
1	B	490	ILE	N-CA	-5.90	1.39	1.46
1	A	340	ASN	C-O	-5.90	1.21	1.23
1	B	527	MET	N-CA	5.89	1.51	1.46
1	B	226	VAL	CA-C	5.89	1.58	1.53
1	B	106	ARG	NE-CZ	5.88	1.39	1.33
1	B	159	ASP	CA-C	5.88	1.60	1.53
1	B	355	GLN	CA-CB	5.87	1.62	1.53
1	A	553	ILE	CA-CB	5.86	1.62	1.54
1	B	290	CYS	CA-CB	5.84	1.62	1.53
1	B	57	LEU	C-O	5.79	1.30	1.23
1	A	77	VAL	CA-CB	-5.77	1.47	1.54
1	B	582	ASP	CA-C	5.77	1.60	1.52
1	A	595	ALA	CA-CB	-5.77	1.44	1.53
1	A	345	GLU	N-CA	-5.76	1.39	1.46
1	B	365	TYR	C-O	5.74	1.31	1.24
1	B	425	HIS	CA-C	-5.73	1.45	1.53
1	B	40	ARG	CG-CD	5.70	1.69	1.52
1	B	387	VAL	CA-C	-5.69	1.45	1.52
1	B	498	ALA	CA-C	-5.66	1.45	1.52
1	B	147	GLU	CA-C	5.66	1.60	1.52
1	A	197	ALA	CA-CB	5.63	1.59	1.53
1	B	555	LEU	C-O	-5.62	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	548	MET	CB-CG	-5.62	1.35	1.52
1	A	561	ARG	NE-CZ	5.62	1.39	1.33
1	B	236	GLU	C-O	-5.62	1.16	1.23
1	B	110	VAL	C-O	5.62	1.30	1.24
1	B	263	ASP	CG-OD2	5.61	1.36	1.25
1	A	540	SER	CA-C	-5.61	1.45	1.52
1	A	99	LEU	CA-C	5.59	1.59	1.52
1	B	237	LEU	N-CA	-5.56	1.39	1.46
1	A	446	ARG	CA-C	5.56	1.59	1.52
1	B	361	LYS	CG-CD	5.55	1.69	1.52
1	A	465	LEU	CG-CD1	-5.53	1.34	1.52
1	B	474	ALA	CA-C	-5.53	1.45	1.52
1	B	605	PHE	C-O	-5.53	1.17	1.24
1	A	522	ARG	CG-CD	5.52	1.69	1.52
1	B	213	VAL	CA-CB	-5.52	1.47	1.54
1	A	549	ALA	C-O	-5.51	1.16	1.24
1	B	217	VAL	CA-CB	-5.51	1.47	1.54
1	A	456	GLY	C-O	-5.49	1.18	1.23
1	A	368	MET	CA-C	-5.47	1.45	1.52
1	B	282	MET	C-O	5.47	1.30	1.23
1	A	118	LYS	CE-NZ	5.47	1.65	1.49
1	A	138	ASP	CA-C	5.46	1.59	1.52
1	A	264	MET	N-CA	5.45	1.53	1.46
1	A	355	GLN	N-CA	5.44	1.53	1.46
1	A	395	GLN	CA-C	-5.44	1.45	1.52
1	B	432	MET	CG-SD	-5.41	1.67	1.80
1	A	230	ALA	CA-CB	5.40	1.62	1.53
1	B	108	GLU	N-CA	-5.39	1.39	1.46
1	A	376	LEU	CA-C	-5.38	1.46	1.52
1	A	352	CYS	C-O	5.38	1.30	1.24
1	A	357	GLY	C-O	-5.37	1.17	1.24
1	B	340	ASN	CA-C	-5.37	1.50	1.53
1	B	78[A]	CYS	C-O	-5.37	1.17	1.24
1	A	491	PHE	CA-C	-5.37	1.46	1.52
1	B	281	PHE	CA-CB	-5.36	1.44	1.53
1	B	133	SER	C-O	-5.36	1.17	1.24
1	A	344	PHE	CA-C	-5.36	1.46	1.52
1	A	249	THR	CB-CG2	5.35	1.70	1.52
1	B	383	VAL	CA-C	5.35	1.59	1.52
1	A	495	MET	SD-CE	5.35	1.93	1.79
1	B	329	MET	CA-C	-5.34	1.46	1.52
1	B	272	GLU	N-CA	-5.34	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLU	CA-C	-5.33	1.45	1.52
1	A	384	LEU	C-O	-5.33	1.17	1.24
1	B	490	ILE	CA-C	5.32	1.59	1.52
1	A	509	ALA	C-O	-5.32	1.17	1.24
1	A	95	LEU	CA-C	5.32	1.59	1.52
1	A	448	VAL	N-CA	-5.31	1.40	1.46
1	A	386	ARG	N-CA	-5.31	1.39	1.46
1	A	225	ILE	CA-CB	5.31	1.60	1.55
1	A	130	SER	C-O	-5.30	1.16	1.23
1	B	442	ARG	CZ-NH1	5.29	1.40	1.32
1	B	363	HIS	CA-C	-5.29	1.47	1.53
1	B	453	PRO	CA-C	-5.29	1.46	1.52
1	A	53	CYS	C-O	-5.28	1.17	1.24
1	A	269	VAL	C-O	-5.28	1.18	1.24
1	A	361	LYS	C-O	-5.28	1.17	1.24
1	A	423	PRO	C-O	-5.28	1.17	1.23
1	B	495	MET	C-O	-5.27	1.17	1.23
1	A	466	MET	CG-SD	5.27	1.94	1.80
1	B	69	SER	CA-C	-5.27	1.46	1.52
1	B	258	LYS	C-O	-5.26	1.17	1.24
1	B	344	PHE	C-O	-5.26	1.17	1.23
1	B	493	SER	CA-C	-5.25	1.47	1.53
1	B	164	VAL	C-O	5.25	1.30	1.24
1	A	128	ILE	C-O	5.24	1.29	1.24
1	A	549	ALA	CA-CB	-5.24	1.44	1.53
1	B	345	GLU	C-O	-5.23	1.17	1.23
1	A	522	ARG	CB-CG	5.23	1.68	1.52
1	A	275	ALA	C-O	-5.23	1.17	1.24
1	B	612	THR	CA-CB	5.21	1.61	1.53
1	B	412	ALA	CA-C	-5.20	1.46	1.52
1	B	107	GLU	C-O	-5.17	1.18	1.24
1	A	529	HIS	CA-C	-5.17	1.47	1.52
1	B	75	TYR	N-CA	-5.17	1.40	1.46
1	B	393	LEU	CA-CB	-5.17	1.46	1.54
1	A	439	LEU	CA-C	5.16	1.59	1.52
1	B	351	ARG	NE-CZ	-5.15	1.27	1.33
1	B	118	LYS	CA-C	-5.15	1.46	1.52
1	A	92	ARG	CZ-NH1	5.12	1.40	1.32
1	A	92	ARG	CA-C	-5.11	1.45	1.52
1	B	523	ASP	CA-CB	5.11	1.57	1.52
1	A	121	ALA	CA-CB	-5.09	1.45	1.53
1	B	414	ALA	C-O	5.09	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	412	ALA	CA-CB	5.09	1.61	1.53
1	A	346[A]	HIS	C-O	5.09	1.30	1.23
1	A	346[B]	HIS	C-O	5.09	1.30	1.23
1	A	333	ARG	N-CA	-5.09	1.39	1.46
1	B	110	VAL	N-CA	-5.08	1.40	1.46
1	B	74	GLU	N-CA	-5.08	1.40	1.46
1	A	341	PRO	CA-CB	-5.06	1.46	1.53
1	A	264	MET	SD-CE	-5.06	1.67	1.79
1	A	401	THR	C-O	-5.05	1.18	1.24
1	B	446	ARG	NE-CZ	5.05	1.38	1.33
1	B	240	PRO	CA-C	5.03	1.58	1.52
1	B	566	ASN	CA-C	5.02	1.59	1.52
1	A	432	MET	C-O	5.02	1.29	1.24
1	A	457	TRP	CA-C	-5.01	1.46	1.52
1	A	369	VAL	C-O	-5.00	1.18	1.24

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	PRO	CA-C-O	-10.21	109.82	121.36
1	B	102	SER	CA-C-N	9.17	131.30	119.84
1	B	102	SER	C-N-CA	9.17	131.30	119.84
1	B	525	ALA	CA-C-N	-8.80	113.24	122.30
1	B	525	ALA	C-N-CA	-8.80	113.24	122.30
1	A	591	MET	CG-SD-CE	-8.25	82.75	100.90
1	B	268	GLN	N-CA-C	7.84	119.91	111.36
1	B	106	ARG	CG-CD-NE	7.79	129.14	112.00
1	A	89	ASP	N-CA-C	7.51	121.55	112.38
1	A	66	THR	N-CA-C	-7.36	103.34	111.36
1	B	425	HIS	N-CA-C	-7.23	99.26	110.17
1	A	614	LEU	N-CA-C	7.07	118.99	111.28
1	A	441	GLU	N-CA-C	7.06	119.83	111.71
1	A	321	ASP	N-CA-C	-6.92	100.03	110.28
1	B	194	LYS	N-CA-C	-6.88	100.27	109.84
1	B	541	HIS	N-CA-C	6.88	119.80	111.82
1	A	40	ARG	N-CA-C	-6.85	103.81	111.28
1	B	225	ILE	N-CA-C	-6.82	105.95	111.81
1	B	92	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	B	103	PRO	N-CA-C	6.72	126.32	112.47
1	B	549	ALA	N-CA-C	6.71	118.36	109.83
1	B	468	ARG	NE-CZ-NH1	-6.60	114.90	121.50
1	A	108	GLU	N-CA-C	6.55	118.42	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	A	285	ARG	N-CA-CB	-6.37	100.75	110.12
1	A	525	ALA	CA-C-N	-6.33	115.78	122.30
1	A	525	ALA	C-N-CA	-6.33	115.78	122.30
1	A	404	LYS	CD-CE-NZ	6.33	132.15	111.90
1	B	264	MET	N-CA-C	-6.30	104.51	111.82
1	A	337	ILE	N-CA-CB	-6.28	102.75	111.41
1	A	541	HIS	N-CA-C	6.18	118.09	111.36
1	A	554	THR	N-CA-C	6.09	120.21	113.21
1	A	138	ASP	N-CA-C	6.08	117.57	111.07
1	B	40	ARG	NE-CZ-NH1	-6.05	115.45	121.50
1	A	358	THR	OG1-CB-CG2	-6.01	97.28	109.30
1	B	523	ASP	CA-C-O	6.00	124.61	120.47
1	A	507	CYS	N-CA-C	5.99	117.50	110.97
1	A	403	LEU	N-CA-C	-5.98	104.68	111.14
1	A	369	VAL	CB-CA-C	-5.97	104.08	112.14
1	B	40	ARG	CB-CG-CD	5.96	125.02	111.30
1	B	523	ASP	CB-CA-C	5.95	116.31	110.71
1	A	70	MET	CB-CA-C	-5.86	101.68	110.88
1	B	408	LYS	N-CA-C	-5.85	104.26	111.40
1	B	334	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	A	47	ARG	N-CA-C	5.83	120.56	112.45
1	B	390	ASN	CB-CA-C	-5.83	103.70	111.63
1	B	40	ARG	NE-CZ-NH2	5.83	124.44	119.20
1	B	550	PRO	CA-C-O	-5.83	114.62	122.08
1	B	419	GLN	N-CA-C	-5.81	101.02	110.20
1	A	472	HIS	N-CA-C	-5.79	105.05	111.36
1	B	482	ASN	N-CA-C	5.78	117.97	109.42
1	B	264	MET	CG-SD-CE	-5.76	88.22	100.90
1	B	54	THR	OG1-CB-CG2	-5.71	97.89	109.30
1	B	291	LEU	N-CA-C	5.68	117.55	111.36
1	A	586	ILE	N-CA-CB	-5.66	104.87	111.83
1	A	49	GLY	N-CA-C	-5.65	104.61	112.18
1	A	66	THR	OG1-CB-CG2	-5.63	98.04	109.30
1	A	557	ILE	CB-CA-C	-5.60	103.87	111.15
1	B	40	ARG	CB-CA-C	5.54	119.99	110.79
1	A	244	LEU	N-CA-C	5.53	117.16	111.03
1	B	341	PRO	CA-C-O	-5.50	115.15	121.86
1	A	363	HIS	N-CA-C	-5.46	101.47	109.50
1	B	183	LYS	N-CA-C	5.46	122.43	110.80
1	A	267	VAL	N-CA-C	-5.45	105.06	110.62
1	B	106	ARG	N-CA-CB	-5.44	102.12	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	CB-CG-CD	5.44	123.81	111.30
1	A	428	HIS	N-CA-C	-5.43	105.26	111.07
1	B	407	PHE	N-CA-C	-5.41	105.55	111.82
1	B	424	VAL	CB-CA-C	-5.40	104.76	111.08
1	B	460	ASP	CB-CA-C	-5.39	101.52	110.68
1	B	431	LEU	N-CA-C	-5.36	105.44	111.28
1	A	285	ARG	CG-CD-NE	-5.35	100.22	112.00
1	A	49	GLY	CA-C-O	-5.35	117.71	121.88
1	B	571	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	B	190	SER	N-CA-C	5.33	118.35	110.46
1	A	334	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	B	397	ARG	N-CA-C	-5.31	102.22	109.71
1	A	354	ARG	CA-C-O	-5.31	114.79	120.42
1	A	449	LEU	CA-C-O	5.30	126.16	120.38
1	B	508	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	595	ALA	CA-C-N	5.27	129.03	120.60
1	A	595	ALA	C-N-CA	5.27	129.03	120.60
1	A	230	ALA	N-CA-C	5.26	122.01	110.80
1	A	98	ASN	N-CA-C	-5.24	106.75	112.72
1	B	521	GLY	N-CA-C	5.23	119.14	112.13
1	A	538	GLU	N-CA-C	-5.23	103.06	109.65
1	B	384	LEU	CA-C-O	5.23	122.74	119.55
1	A	60	LEU	N-CA-C	5.20	117.03	111.36
1	B	102	SER	CA-C-O	-5.20	113.04	120.16
1	B	374	ASP	N-CA-CB	-5.19	102.50	110.44
1	A	460	ASP	CA-C-N	-5.17	113.66	122.56
1	A	460	ASP	C-N-CA	-5.17	113.66	122.56
1	A	265	GLN	N-CA-C	5.15	116.90	111.28
1	B	161	PRO	CA-C-O	5.13	127.92	121.67
1	A	572	MET	N-CA-C	-5.12	101.61	109.76
1	B	328	LEU	CB-CA-C	-5.11	101.31	109.75
1	B	416[A]	SER	CB-CA-C	-5.05	100.28	109.38
1	B	416[B]	SER	CB-CA-C	-5.05	100.28	109.38
1	B	354	ARG	N-CA-C	5.05	117.68	111.82
1	B	79	HIS	N-CA-C	5.05	118.27	112.57

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

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Mol	Chain	Res	Type	Group
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	103	0
1	B	4717	0	4653	137	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	28	0
All	All	10000	0	9121	235	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 13.

All (235) 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:CG1	1:B:553:ILE:CD1	1.75	1.63
1:B:466:MET:CE	1:B:466:MET:SD	2.04	1.46
1:A:466:MET:CE	1:A:466:MET:SD	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:A:241:GLU:H	1:A:241:GLU:CD	1.66	1.01
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: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: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:102:SER:C	4:B:3108:HOH:O	2.21	0.83
1:B:103:PRO:N	4:B:3108:HOH:O	2.11	0.83
1:B:241:GLU:H	1:B:241:GLU:CD	1.86	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:B:241:GLU:CD	1:B:241:GLU:N	2.39	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:A:235:LYS:HZ3	1:A:279:ASN:HD21	1.29	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: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:161:PRO:C	4:A:3215:HOH:O	2.32	0.72
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:A:241:GLU:CD	1:A:241:GLU:N	2.42	0.71
1:B:578:GLU:C	1:B:579:HIS:CG	2.69	0.70
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:89:ASP:C	4:A:3209:HOH:O	2.36	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: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:66:THR:HG23	1:A:70:MET:HE2	1.79	0.62
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:75:TYR:C	1:A:75:TYR:CD1	2.77	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:B:468:ARG:HD2	4:B:2817:HOH:O	2.00	0.60
1:A:79:HIS:CG	4:A:3208:HOH:O	2.55	0.60
1:B:179:ALA:C	1:B:180:GLY:O	2.45	0.60
1:A:370:MET:HE3	1:A:370:MET:HA	1.82	0.60
1:B:607:ALA:HA	4:B:3116:HOH:O	2.01	0.59
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:184:GLY:HA2	1:B:189:ASP:CB	2.32	0.59
1:A:371:GLU:HG3	4:A:3133:HOH:O	2.02	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:CE	1:B:466:MET:CG	2.82	0.58
1:A:214:GLN:HG2	4:A:3197:HOH:O	2.04	0.58
1:A:596:ARG:CG	4:A:3231:HOH:O	2.41	0.57
1:B:112:ARG:O	1:B:116:VAL:HG23	2.06	0.56
1:B:64:GLY:HA2	2:B:2800:ADP:H5'1	1.87	0.56
1:B:184:GLY:O	1:B:190:SER:OG	2.19	0.55
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:B:40:ARG:CB	1:B:40:ARG:HH11	2.20	0.54
1:A:231:SER:OG	1:A:404:LYS:HE2	2.08	0.54
1:B:235:LYS:NZ	1:B:279:ASN:OD1	2.40	0.54
1:A:382:GLN:CD	4:A:3227:HOH:O	2.51	0.54
1:A:235:LYS:HZ2	1:A:279:ASN:ND2	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLU:O	1:B:234:VAL:C	2.48	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
1:B:166:GLU:HG2	1:B:174:TYR:CG	2.44	0.52
1:A:579:HIS:O	1:A:580:HIS:C	2.52	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:B:545:VAL:CG2	1:A:292[A]:HIS:HD2	2.22	0.52
1:A:314:HIS:HD2	1:A:375:TRP:HE1	1.58	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:B:106:ARG:HD2	3:B:2805:ADX:O1B	2.09	0.51
1:A:340:ASN:N	1:A:341:PRO:CD	2.73	0.51
1:B:340:ASN:N	1:B:341:PRO:HD3	2.26	0.51
3:B:2805:ADX:N3	3:B:2805:ADX:C2'	2.71	0.51
1:B:579:HIS:O	1:B:580:HIS:C	2.53	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:579:HIS:C	1:B:581:GLU:N	2.67	0.51
1:A:416[B]:SER:HB3	4:A:3233:HOH:O	2.11	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:B:491:PHE:CE2	1:B:493:SER:HB3	2.47	0.49
1:A:96:ASN:ND2	1:A:109:ASN:OD1	2.45	0.49
1:B:450:LEU:HD21	1:B:452:HIS:ND1	2.26	0.49
1:A:42:GLN:NE2	4:A:3185:HOH:O	2.44	0.49
1:A:363:HIS:HB3	1:A:366:ILE:HB	1.93	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:476:LEU:HD23	1:B:481:LEU:O	2.14	0.47
1:A:79:HIS:CE1	4:A:3208:HOH:O	2.66	0.47
1:A:231:SER:OG	1:A:404:LYS:CE	2.62	0.47
1:A:420:LEU:HD13	1:A:453:PRO:HA	1.96	0.47
1:B:108:GLU:HA	1:B:108:GLU:OE1	2.13	0.47
1:B:622:GLU:O	1:B:623:LYS:HG3	2.14	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:101:PHE:HB2	1:B:183:LYS:HD3	1.95	0.47
1:B:40:ARG:HH11	1:B:40:ARG:CG	2.27	0.47
1:A:356:TRP:CD1	1:A:498:ALA:HB2	2.50	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:CE	1:A:466:MET:CG	2.91	0.46
1:B:186:THR:HG23	3:B:2805:ADX:H2	1.97	0.46
1:B:75:TYR:OH	4:B:3117:HOH:O	2.19	0.46
1:B:596:ARG:C	1:B:598:GLY:H	2.24	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:B:465:LEU:O	1:B:466:MET:C	2.59	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:83:CYS:HA	1:A:126:VAL:O	2.17	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:B:123:ALA:HB2	1:A:84:TYR:CD1	2.52	0.44
1:A:330:TYR:OH	4:A:3190:HOH:O	2.21	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:395:GLN:H	1:A:395:GLN:CD	2.25	0.44
1:A:386:ARG:HE	1:A:386:ARG:HB3	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346[B]:HIS:HE1	1:A:369:VAL:HG13	1.83	0.44
1:B:579:HIS:C	1:B:581:GLU:H	2.26	0.43
1:B:361:LYS:HE3	4:B:3090:HOH:O	2.18	0.43
1:A:408:LYS:O	1:A:411:ASN:N	2.42	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
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:A:454:LEU:HD23	1:A:454:LEU:C	2.44	0.42
1:B:452:HIS:O	1:B:453:PRO:C	2.62	0.42
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:A:70:MET:CE	1:A:70:MET:CG	2.95	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: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:495:MET:HE1	1:A:525:ALA:HA	2.02	0.42
1:B:386:ARG:HG3	1:B:387:VAL:H	1.83	0.42
1:B:606:MET:O	1:B:607:ALA:C	2.63	0.42
1:A:410[B]:MET:HE2	1:A:448:VAL:HG21	2.02	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: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:B:85:THR:HB	1:A:34:HIS:HE1	1.85	0.41
1:A:511:MET:HB2	1:A:555:LEU:HD13	2.03	0.41
1:B:555:LEU:HD12	1:B:555:LEU:C	2.46	0.41
1:B:239:VAL:HG23	1:B:240:PRO:HD2	2.01	0.41
1:A:196:GLU:CG	4:A:3212:HOH:O	2.68	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:307:PRO:HD2	1:A:355:GLN:CD	2.45	0.41
1:B:161:PRO:O	1:B:162:LEU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:435:THR:O	1:A:439:LEU:HG	2.20	0.41
1:B:51:ARG:NE	1:B:225:ILE:O	2.50	0.41
1:B:545:VAL:CG2	1:A:292[A]:HIS:CD2	2.99	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:A:360:CYS:SG	1:A:530:PRO:HG2	2.60	0.41
1:B:612:THR:O	1:B:613:VAL:C	2.64	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:B:440:LEU:HD23	1:B:444:TYR:O	2.22	0.40
1:B:442:ARG:NH1	4:B:3113:HOH:O	2.54	0.40
1:A:621:LEU:HD23	1:A:621:LEU:HA	1.82	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

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	566/630 (90%)	547 (97%)	17 (3%)	2 (0%)	30	20
1	B	591/630 (94%)	557 (94%)	24 (4%)	10 (2%)	7	1
All	All	1157/1260 (92%)	1104 (95%)	41 (4%)	12 (1%)	12	5

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	SER
1	B	103	PRO
1	B	183	LYS

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Mol	Chain	Res	Type
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%)	450 (92%)	39 (8%)	11	3
1	B	507/538 (94%)	458 (90%)	49 (10%)	8	1
All	All	996/1076 (93%)	908 (91%)	88 (9%)	9	2

All (88) 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	167	GLN
1	B	171	LYS
1	B	173	LEU
1	B	176	LYS
1	B	182	ILE

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Mol	Chain	Res	Type
1	B	186	THR
1	B	196	GLU
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
1	B	446	ARG
1	B	472	HIS
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	569	LYS
1	B	570	LYS
1	B	571	ARG
1	B	577	SER
1	B	578	GLU
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	620	SER
1	B	621	LEU
1	B	622	GLU
1	A	34	HIS
1	A	39	LYS
1	A	40	ARG
1	A	42	GLN
1	A	46	THR
1	A	47	ARG
1	A	54	THR

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Mol	Chain	Res	Type
1	A	66	THR
1	A	70	MET
1	A	82	PRO
1	A	93	GLN
1	A	118	LYS
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	347	ARG
1	A	386	ARG
1	A	420	LEU
1	A	441	GLU
1	A	445	ARG
1	A	508	ARG
1	A	522	ARG
1	A	534	LYS
1	A	553	ILE
1	A	568	LYS
1	A	570	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	ASN
1	B	109	ASN
1	B	141	ASN
1	B	144	GLN
1	B	163	HIS
1	B	210	ASN

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Mol	Chain	Res	Type
1	B	346	HIS
1	B	411	ASN
1	B	422	ASN
1	B	425	HIS
1	B	436	HIS
1	B	599	GLN
1	A	42	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	ADP	B	2800	-	28,29,29	1.57	3 (10%)	43,45,45	2.11	14 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADX	B	2700	-	29,29,29	1.82	7 (24%)	42,45,45	3.05	19 (45%)
3	ADX	A	2900	-	29,29,29	1.81	7 (24%)	42,45,45	2.32	15 (35%)
3	ADX	B	2805	-	29,29,29	1.46	5 (17%)	42,45,45	2.93	19 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	2800	-	-	2/16/32/32	0/3/3/3
3	ADX	B	2700	-	-	2/10/32/32	0/3/3/3
3	ADX	A	2900	-	-	2/10/32/32	0/3/3/3
3	ADX	B	2805	-	-	3/10/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2900	ADX	C8-N7	4.36	1.40	1.31
2	B	2800	ADP	C8-N7	4.36	1.40	1.31
3	B	2700	ADX	C8-N7	4.20	1.39	1.31
3	B	2700	ADX	C2-N1	3.99	1.41	1.33
3	A	2900	ADX	C8-N9	3.57	1.43	1.37
3	B	2700	ADX	PA-O1A	-3.44	1.38	1.50
3	A	2900	ADX	O2'-C2'	-3.23	1.35	1.43
3	B	2805	ADX	O2B-SB	3.22	1.59	1.45
3	B	2805	ADX	C2-N1	3.18	1.39	1.33
3	A	2900	ADX	C4-N9	-3.01	1.31	1.37
2	B	2800	ADP	C2-N3	2.96	1.39	1.33
2	B	2800	ADP	C4-N9	2.82	1.43	1.37
3	B	2700	ADX	C3'-C4'	2.66	1.59	1.53
3	B	2700	ADX	PA-O5'	-2.56	1.49	1.59
3	A	2900	ADX	PA-O5'	-2.54	1.49	1.59
3	A	2900	ADX	O4'-C1'	2.49	1.47	1.42
3	B	2805	ADX	C6-N1	2.48	1.42	1.35
3	B	2805	ADX	C2-N3	2.44	1.38	1.33
3	B	2805	ADX	C8-N7	2.28	1.36	1.31
3	A	2900	ADX	C2-N3	2.22	1.37	1.33
3	B	2700	ADX	C5-C6	-2.10	1.35	1.41
3	B	2700	ADX	C5-N7	-2.04	1.35	1.39

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2700	ADX	O3B-SB-O2B	8.70	139.01	108.56
3	B	2805	ADX	N3-C2-N1	-7.90	116.63	128.58
3	A	2900	ADX	N3-C2-N1	-7.32	117.50	128.58
3	B	2700	ADX	O3B-SB-O3A	-6.83	91.38	106.02
3	B	2805	ADX	N9-C8-N7	-6.80	104.29	113.94
3	B	2700	ADX	O5'-PA-O3A	6.63	123.15	103.09
3	B	2700	ADX	N9-C8-N7	-6.16	105.19	113.94
2	B	2800	ADP	N9-C8-N7	-5.40	106.28	113.94
2	B	2800	ADP	O2A-PA-O3A	5.33	121.67	107.27
3	B	2805	ADX	C4-N9-C8	5.13	111.12	105.74
3	B	2805	ADX	C5-N7-C8	5.04	111.38	103.45
3	B	2700	ADX	N3-C2-N1	-5.03	120.97	128.58
2	B	2800	ADP	N3-C2-N1	-4.92	121.14	128.58
3	B	2805	ADX	C5-C4-N3	-4.81	120.10	126.72
3	A	2900	ADX	N9-C8-N7	-4.80	107.13	113.94
3	B	2805	ADX	C2-N3-C4	4.75	123.43	111.83
3	A	2900	ADX	O4'-C1'-N9	-4.62	99.22	108.09
3	B	2805	ADX	N3-C4-N9	4.42	134.69	127.17
3	B	2700	ADX	C5-N7-C8	4.36	110.30	103.45
3	B	2805	ADX	C5-C6-N6	-4.27	112.71	123.29
3	B	2700	ADX	C4-N9-C8	4.21	110.16	105.74
3	A	2900	ADX	C2-N1-C6	4.15	125.55	118.73
2	B	2800	ADP	C5-N7-C8	4.04	109.80	103.45
3	B	2700	ADX	O4'-C1'-N9	-3.97	100.46	108.09
3	B	2805	ADX	C3'-C2'-C1'	3.93	108.90	101.46
3	B	2805	ADX	O2B-SB-O1B	-3.78	97.66	112.24
3	B	2700	ADX	O2'-C2'-C3'	3.61	123.40	111.82
3	B	2700	ADX	C6-C5-C4	3.51	121.98	117.18
3	A	2900	ADX	O3B-SB-O2B	3.50	120.81	108.56
2	B	2800	ADP	O2A-PA-O5'	3.36	122.78	107.57
2	B	2800	ADP	C4-N9-C8	3.31	109.21	105.74
3	B	2805	ADX	O4'-C1'-N9	3.02	113.89	108.09
2	B	2800	ADP	C5-C4-N3	-2.96	122.64	126.72
2	B	2800	ADP	O2A-PA-O1A	-2.95	98.71	112.44
3	A	2900	ADX	C5-C4-N9	2.92	109.00	105.81
3	B	2805	ADX	O2A-PA-O5'	2.80	120.25	107.57
3	B	2700	ADX	C2'-C1'-N9	2.76	120.16	113.30
3	B	2805	ADX	O3B-SB-O2B	2.76	118.20	108.56
3	A	2900	ADX	C4-N9-C8	2.74	108.62	105.74
3	B	2805	ADX	N6-C6-N1	2.74	124.47	118.38
3	B	2700	ADX	C5-C4-N3	-2.72	122.97	126.72
3	A	2900	ADX	O4'-C1'-C2'	-2.72	100.80	106.62

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2800	ADP	O3A-PA-O1A	-2.69	102.62	110.70
3	B	2805	ADX	O4'-C1'-C2'	-2.68	100.89	106.62
3	B	2700	ADX	C5-C6-N6	-2.67	116.68	123.29
3	B	2700	ADX	O2'-C2'-C1'	-2.67	100.92	110.10
3	B	2805	ADX	O3'-C3'-C4'	2.66	118.72	111.08
3	A	2900	ADX	O2B-SB-O1B	-2.63	102.08	112.24
3	B	2700	ADX	C4-C5-N7	-2.62	107.59	110.58
3	B	2700	ADX	O2A-PA-O3A	-2.58	100.31	107.27
3	A	2900	ADX	O2A-PA-O3A	-2.54	100.41	107.27
3	A	2900	ADX	C2-N3-C4	2.53	118.01	111.83
3	B	2700	ADX	O5'-C5'-C4'	2.50	117.51	108.99
3	A	2900	ADX	C5-N7-C8	2.35	107.15	103.45
3	B	2700	ADX	O3'-C3'-C2'	-2.32	104.37	111.82
3	B	2805	ADX	C4-C5-N7	-2.28	107.98	110.58
2	B	2800	ADP	N3-C4-N9	2.24	130.98	127.17
2	B	2800	ADP	O2B-PB-O3A	2.24	112.14	104.64
3	A	2900	ADX	C4-C5-N7	-2.22	108.05	110.58
2	B	2800	ADP	O4'-C1'-N9	2.19	112.30	108.09
3	B	2805	ADX	O5'-PA-O3A	-2.10	96.72	103.09
3	A	2900	ADX	O4'-C4'-C5'	2.09	116.02	109.33
3	A	2900	ADX	O3B-SB-O3A	2.05	110.41	106.02
2	B	2800	ADP	C2-N1-C6	2.05	122.09	118.73
3	B	2805	ADX	O4'-C4'-C3'	2.04	109.20	105.15
2	B	2800	ADP	C4-C5-N7	-2.04	108.25	110.58
3	B	2700	ADX	C2-N3-C4	2.02	116.77	111.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

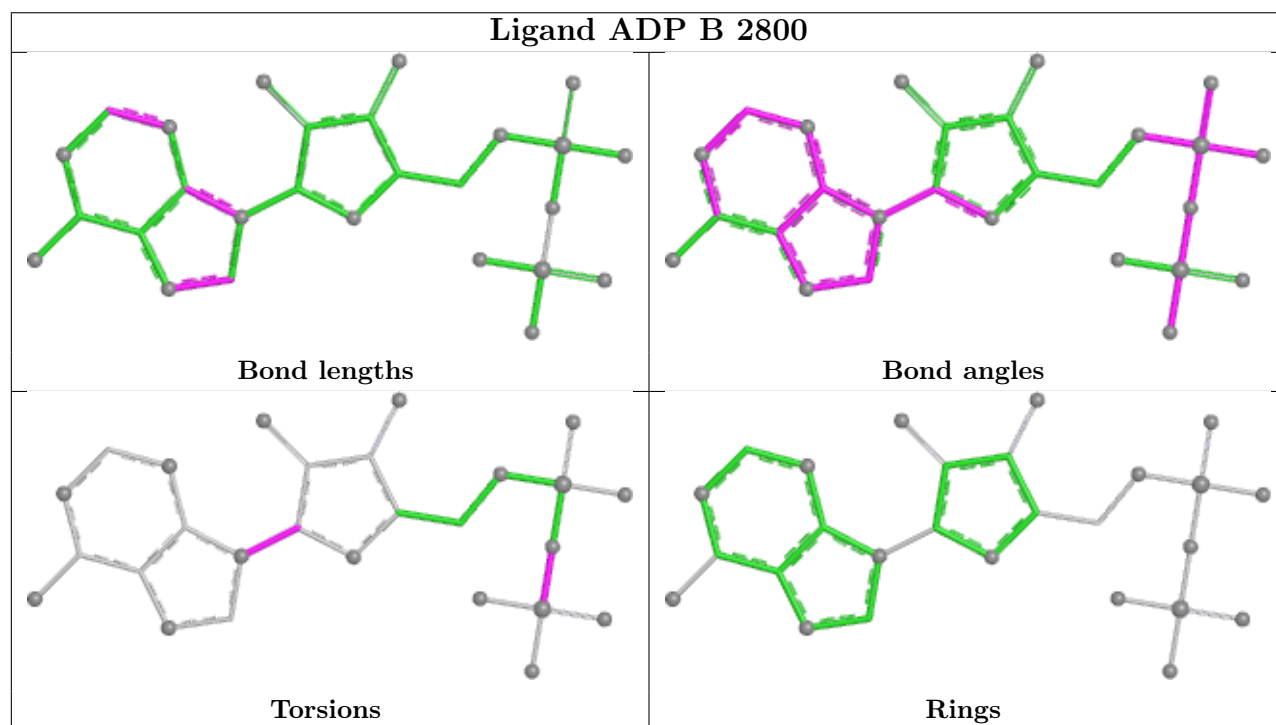
Mol	Chain	Res	Type	Atoms
3	B	2805	ADX	C5'-O5'-PA-O1A
3	A	2900	ADX	C5'-O5'-PA-O1A
3	A	2900	ADX	C5'-O5'-PA-O3A
3	B	2805	ADX	C2'-C1'-N9-C4
3	B	2805	ADX	C2'-C1'-N9-C8
2	B	2800	ADP	PA-O3A-PB-O1B
3	B	2700	ADX	O4'-C4'-C5'-O5'
3	B	2700	ADX	C3'-C4'-C5'-O5'
2	B	2800	ADP	O4'-C1'-N9-C8

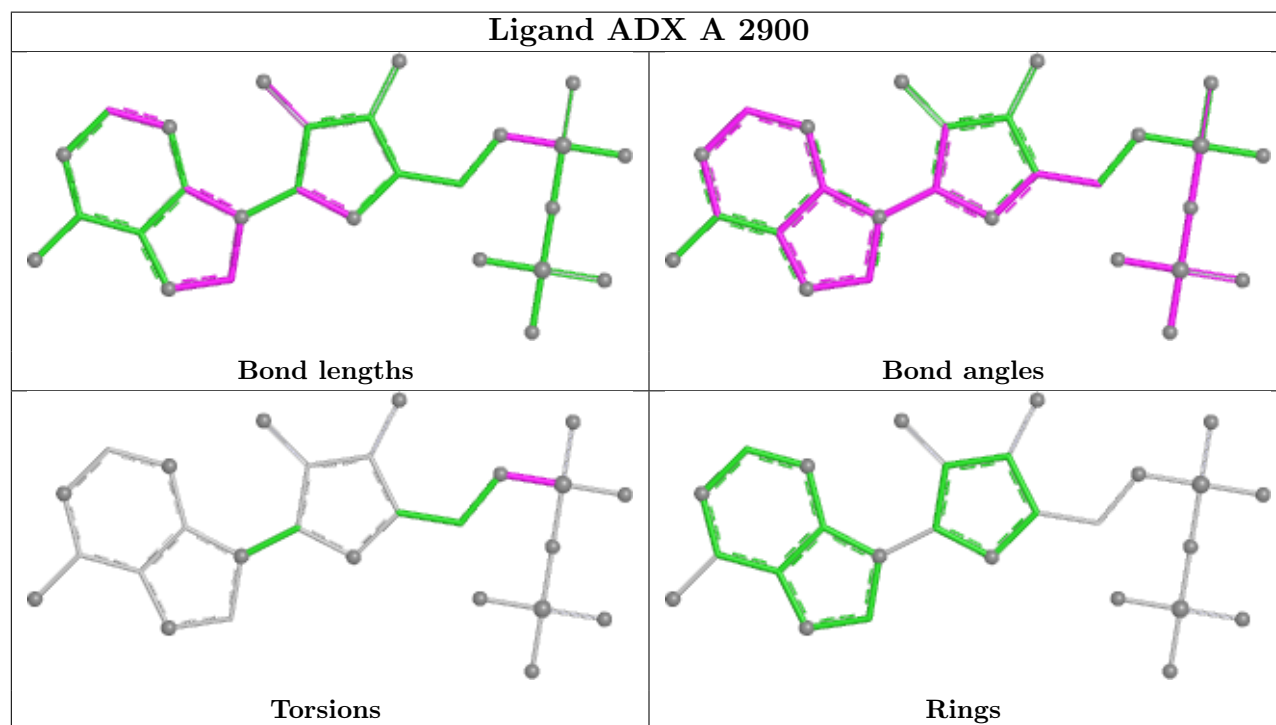
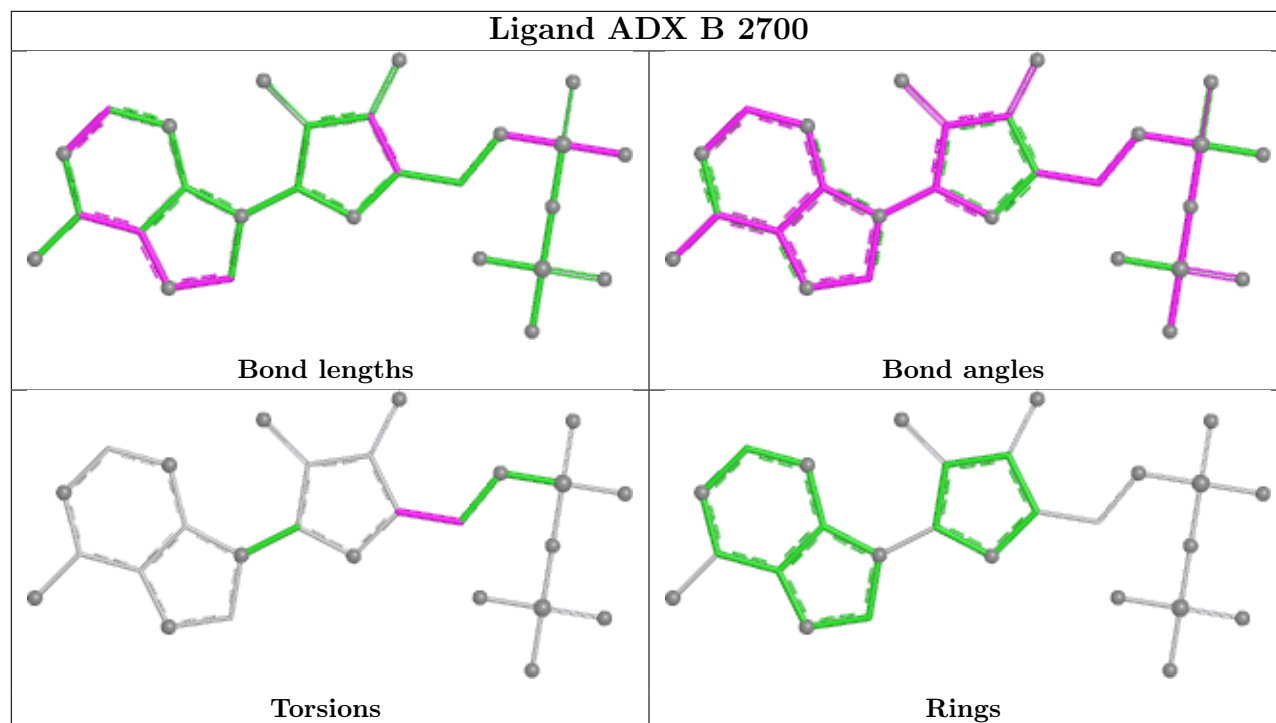
There are no ring outliers.

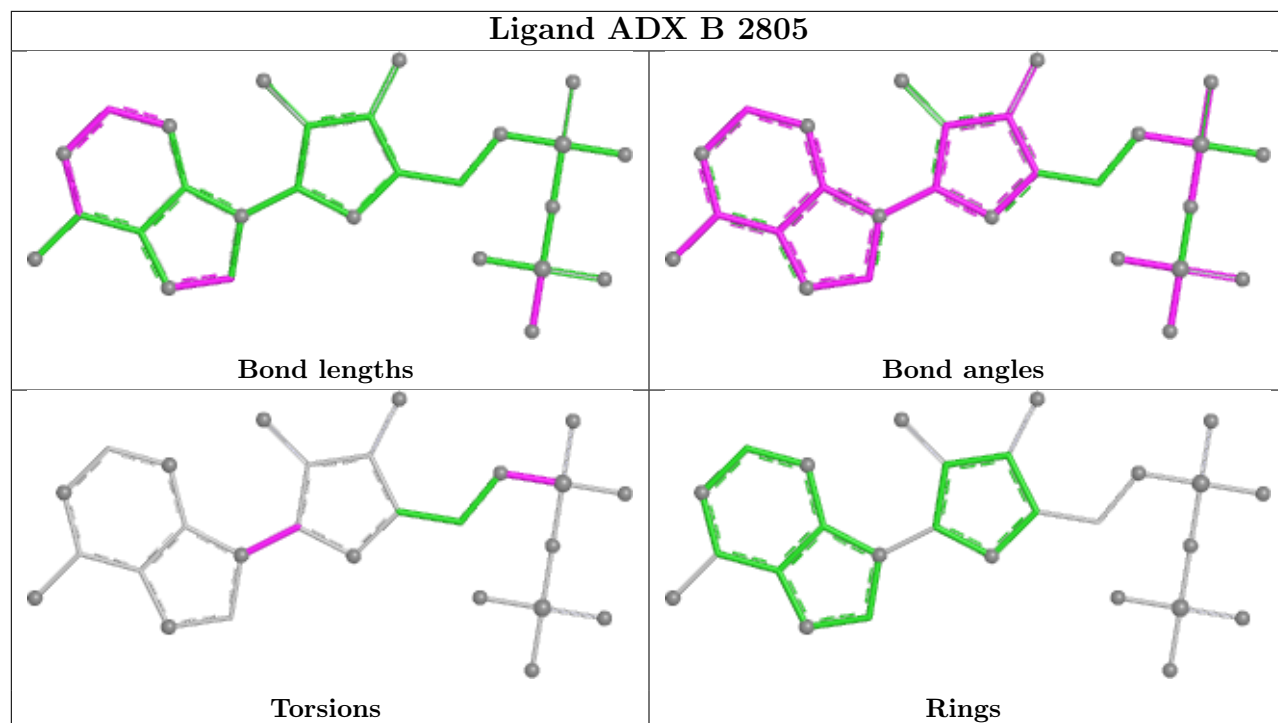
2 monomers are involved in 7 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.03	12 (2%) 63 72	14, 34, 60, 82	10 (1%)
1	B	590/630 (93%)	0.15	6 (1%) 79 86	14, 36, 65, 88	3 (0%)
All	All	1152/1260 (91%)	0.09	18 (1%) 70 79	14, 35, 63, 88	13 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	TYR	4.8
1	A	46	THR	3.9
1	A	34	HIS	3.4
1	A	230	ALA	3.1
1	A	161	PRO	3.0
1	B	179	ALA	2.9
1	A	47	ARG	2.6
1	B	565	TYR	2.4
1	B	580	HIS	2.3
1	B	577	SER	2.2
1	A	228	VAL	2.2
1	A	45	GLY	2.2
1	A	436	HIS	2.2
1	B	623	LYS	2.2
1	A	49	GLY	2.1
1	B	197	ALA	2.1
1	A	441	GLU	2.0
1	A	245	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

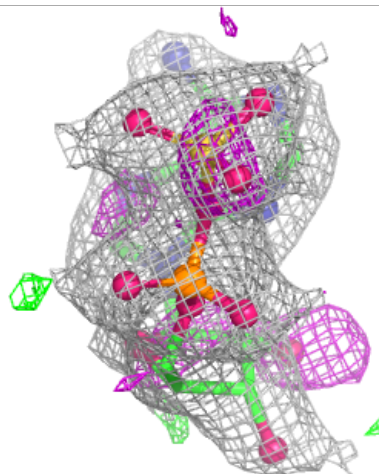
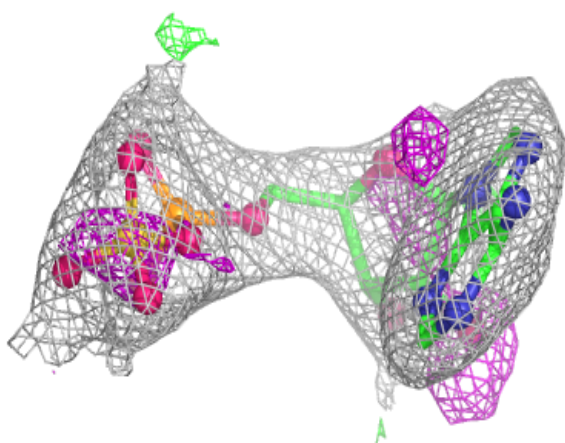
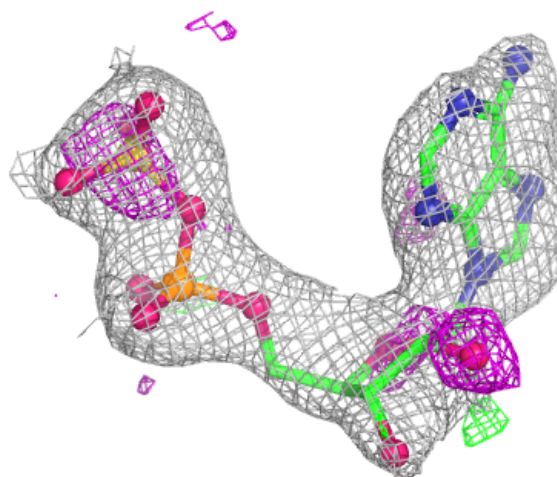
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADX	B	2805	27/27	0.93	0.10	49,61,71,73	0
2	ADP	B	2800	27/27	0.96	0.07	40,46,48,52	0
3	ADX	B	2700	27/27	0.98	0.05	28,34,41,42	0
3	ADX	A	2900	27/27	0.99	0.04	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.

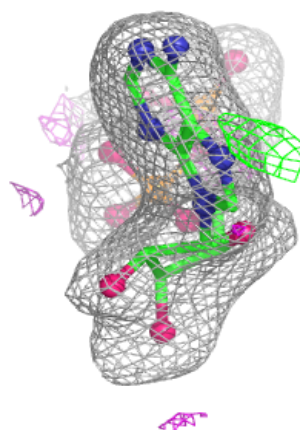
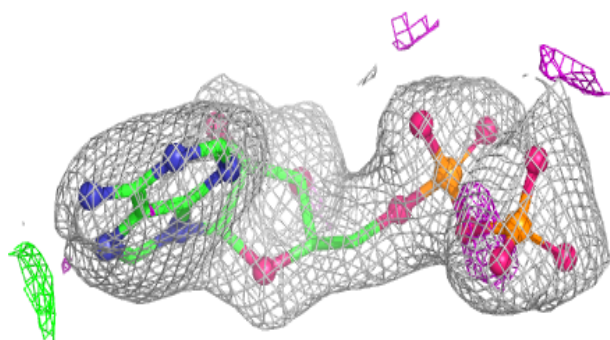
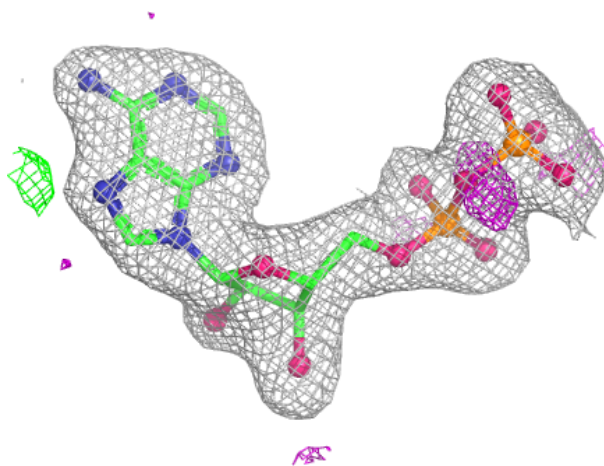
Electron density around ADX B 2805:

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



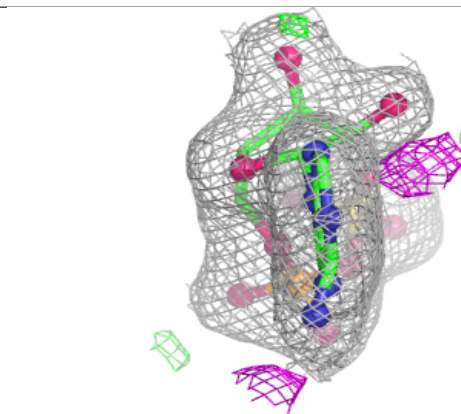
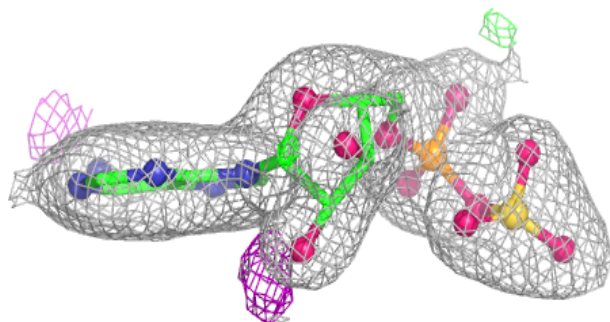
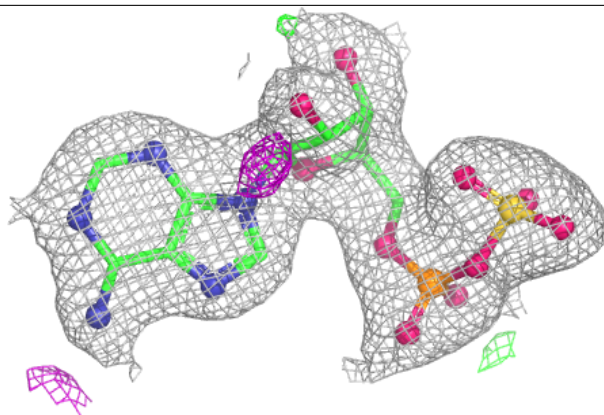
Electron density around ADP B 2800:

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

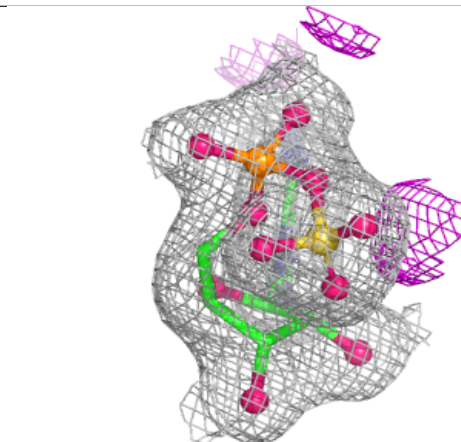
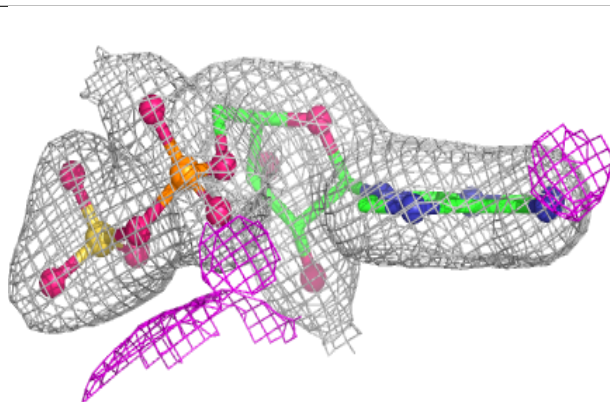
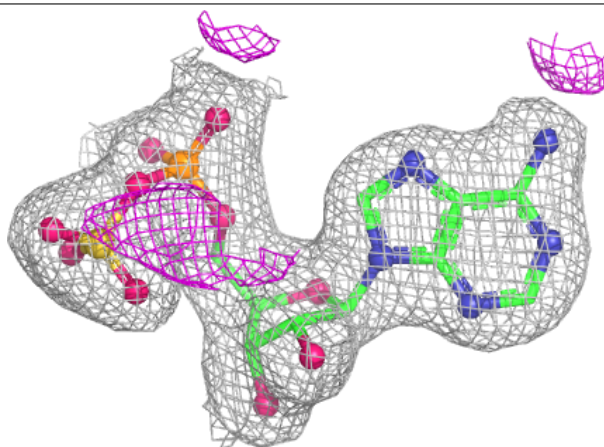


Electron density around ADX B 2700:

$2mF_o-DF_c$ (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.