



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:23 AM UTC

PDB ID : 1G8H / pdb_00001g8h
Title : ATP SULFURYLASE FROM S. CEREVISIAE: THE TERNARY PRODUCT
COMPLEX WITH APS AND PPI
Authors : Ullrich, T.C.; Blaesse, M.; Huber, R.
Deposited on : 2000-11-17
Resolution : 2.80 Å(reported)

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

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

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

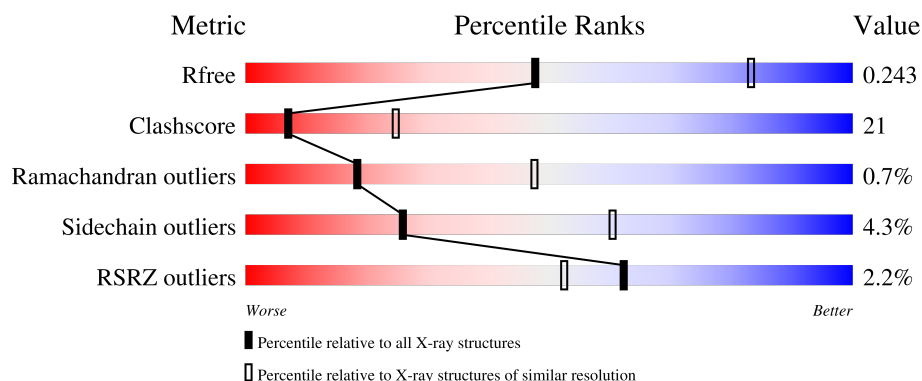
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	511	3% 63% 33% .
1	B	511	% 63% 33% .

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8917 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 SULFATE ADENYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4077	2598	707	767	5			
1	B	510	Total	C	N	O	S	0	0	0
			4077	2598	707	767	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	ARG	LYS	conflict	UNP P08536
A	457	ASP	ASN	conflict	UNP P08536
B	131	ARG	LYS	conflict	UNP P08536
B	457	ASP	ASN	conflict	UNP P08536

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Cd	0	0
			6	6		
2	B	5	Total	Cd	0	0
			5	5		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		
3	B	3	Total	Ca	0	0
			3	3		

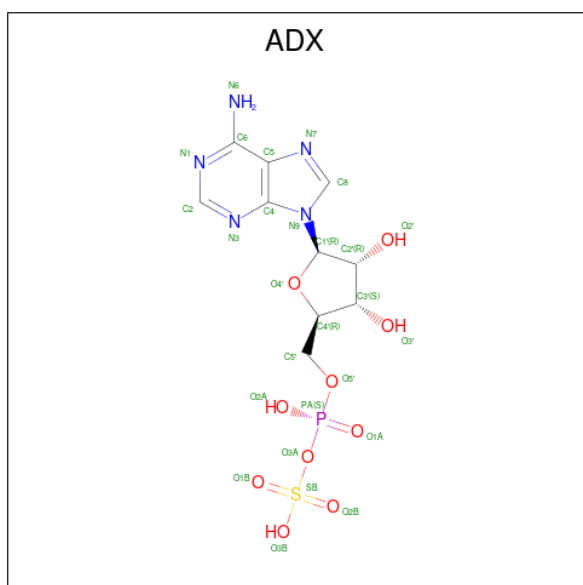
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total Na 6 6	0	0
4	B	6	Total Na 6 6	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

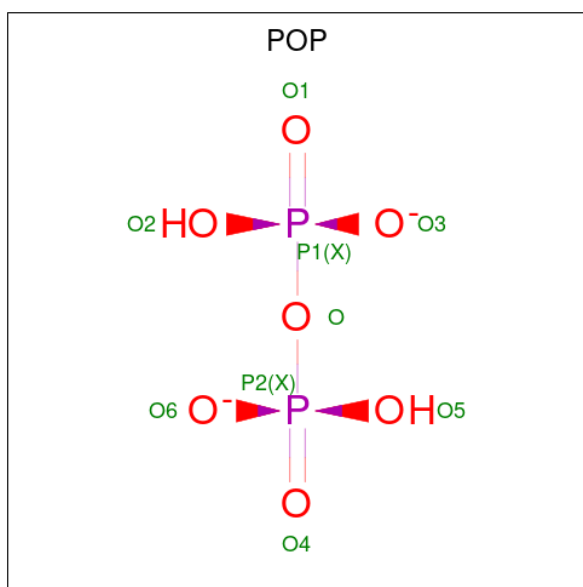
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is ADENOSINE-5'-PHOSPHOSULFATE (CCD ID: ADX) (formula: C₁₀H₁₄N₅O₁₀PS).



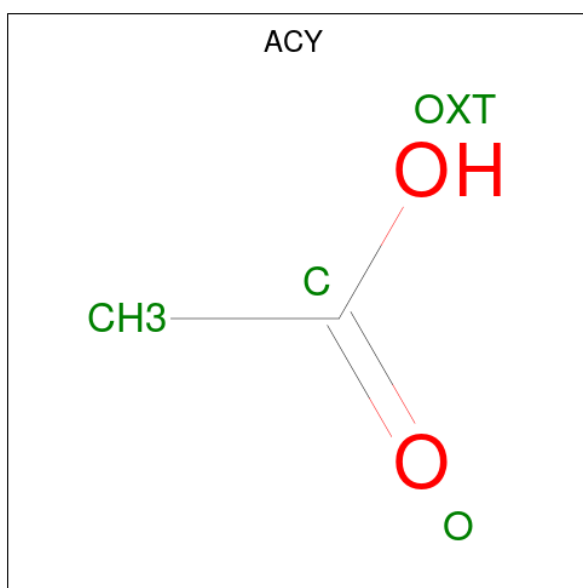
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P S 27 10 5 10 1 1	0	0
6	B	1	Total C N O P S 27 10 5 10 1 1	0	0

- Molecule 7 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			9	7	2		
7	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 8 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		

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

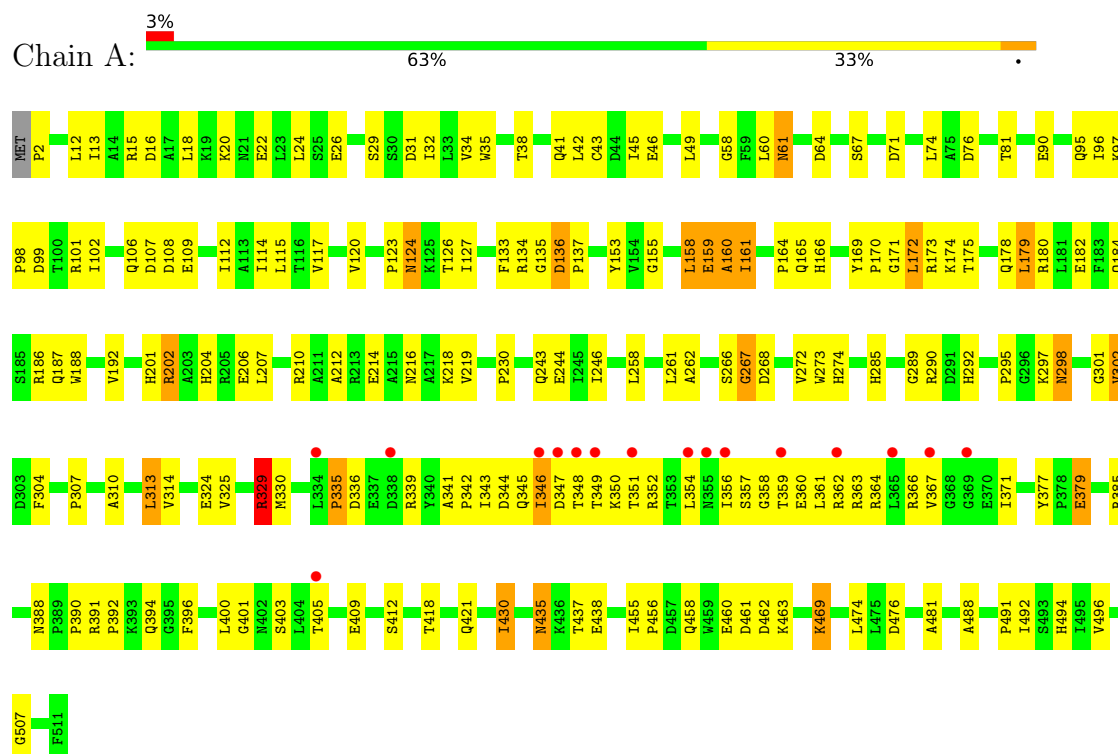
- Molecule 9 is water.

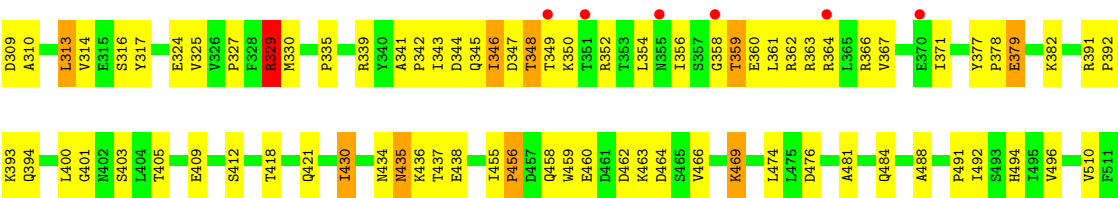
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	301	Total O 301 301	0	0
9	B	299	Total O 299 299	0	0

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: SULFATE ADENYLYLTRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	186.01Å 186.01Å 223.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.87 – 2.80 24.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (24.87-2.80) 95.2 (24.87-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.245 0.194 , 0.243	Depositor DCC
R_{free} test set	1801 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.018 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.012 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8917	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.46% 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: NA, POP, CA, CD, MG, ACY, ADX

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	0.44	0/4173	0.95	22/5670 (0.4%)
1	B	0.44	0/4173	0.95	18/5670 (0.3%)
All	All	0.44	0/8346	0.95	40/11340 (0.4%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	ILE	N-CA-C	-8.41	97.78	108.89
1	B	430	ILE	N-CA-C	-8.38	97.83	108.89
1	B	161	ILE	N-CA-C	-8.19	105.27	111.90
1	A	161	ILE	N-CA-C	-7.54	105.32	111.81
1	B	81	THR	N-CA-C	7.03	121.94	113.23
1	A	388	ASN	CA-C-N	6.52	124.42	119.66
1	A	388	ASN	C-N-CA	6.52	124.42	119.66
1	A	81	THR	N-CA-C	6.47	121.37	112.90
1	A	371	ILE	CA-C-N	6.37	126.40	119.90
1	A	371	ILE	C-N-CA	6.37	126.40	119.90
1	B	13	ILE	N-CA-C	-6.21	104.69	110.53
1	B	60	LEU	N-CA-C	5.96	119.00	110.24
1	B	371	ILE	CA-C-N	5.88	127.19	119.84
1	B	371	ILE	C-N-CA	5.88	127.19	119.84
1	A	74	LEU	N-CA-C	-5.87	102.63	110.55
1	A	172	LEU	N-CA-C	5.72	119.99	112.89
1	A	13	ILE	N-CA-C	-5.69	104.97	110.72
1	B	135	GLY	N-CA-C	5.68	126.65	113.18
1	B	160	ALA	N-CA-C	5.54	118.48	110.28
1	B	34	VAL	N-CA-C	5.50	116.40	108.48
1	A	60	LEU	N-CA-C	5.50	118.32	110.24
1	B	172	LEU	N-CA-C	5.46	120.00	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	GLY	N-CA-C	5.45	126.10	113.18
1	A	136	ASP	CA-C-N	5.29	124.95	119.56
1	A	136	ASP	C-N-CA	5.29	124.95	119.56
1	A	117	VAL	N-CA-C	5.26	116.47	109.37
1	A	159	GLU	N-CA-C	-5.26	98.71	107.80
1	A	455	ILE	CA-C-N	5.23	124.89	119.56
1	A	455	ILE	C-N-CA	5.23	124.89	119.56
1	B	74	LEU	N-CA-C	-5.23	103.79	110.53
1	B	304	PHE	N-CA-C	-5.22	105.66	112.23
1	A	507	GLY	N-CA-C	5.20	122.28	115.47
1	B	329	ARG	N-CA-C	-5.17	102.81	110.46
1	A	34	VAL	N-CA-C	5.14	115.88	108.48
1	A	329	ARG	N-CA-C	-5.10	102.92	110.46
1	B	348	THR	N-CA-C	-5.08	107.44	113.38
1	B	117	VAL	N-CA-C	5.08	116.22	109.37
1	B	456	PRO	N-CA-C	5.04	120.40	113.84
1	B	118	GLN	N-CA-C	-5.04	107.20	113.55
1	A	160	ALA	N-CA-C	5.04	118.16	110.20

There are no chirality outliers.

There are no planarity outliers.

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	4077	0	4033	171	0
1	B	4077	0	4033	173	0
2	A	6	0	0	0	1
2	B	5	0	0	0	1
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	13	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	27	0	13	0	0
7	A	9	0	0	1	0
7	B	9	0	0	0	0
8	A	32	0	24	2	0
8	B	28	0	21	2	0
9	A	301	0	0	14	0
9	B	299	0	0	15	0
All	All	8917	0	8137	346	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (346) 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:A:329:ARG:H	1:A:329:ARG:HD2	1.06	1.08
1:B:329:ARG:H	1:B:329:ARG:HD2	1.06	1.06
1:A:106:GLN:HE22	1:A:165:GLN:H	1.12	0.98
1:A:58:GLY:HA2	1:A:158:LEU:HD22	1.48	0.95
1:B:106:GLN:HE22	1:B:165:GLN:H	1.09	0.94
1:A:362:ARG:HB2	1:A:362:ARG:NH1	1.86	0.91
1:B:362:ARG:NH1	1:B:362:ARG:HB2	1.86	0.90
1:B:469:LYS:N	1:B:469:LYS:HE2	1.86	0.90
1:B:329:ARG:HD2	1:B:329:ARG:N	1.87	0.90
1:B:469:LYS:HE2	1:B:469:LYS:H	1.35	0.89
1:A:329:ARG:HD2	1:A:329:ARG:N	1.87	0.89
1:B:58:GLY:HA2	1:B:158:LEU:HD22	1.55	0.88
1:A:469:LYS:HE2	1:A:469:LYS:N	1.94	0.83
1:A:61:ASN:ND2	1:A:64:ASP:H	1.77	0.83
1:B:329:ARG:H	1:B:329:ARG:CD	1.92	0.81
1:B:348:THR:HG21	1:B:350:LYS:HZ2	1.46	0.80
1:A:469:LYS:HE2	1:A:469:LYS:H	1.45	0.80
1:B:412:SER:HB3	1:B:430:ILE:HD12	1.64	0.79
1:A:175:THR:H	1:A:178:GLN:HE21	1.27	0.78
1:A:348:THR:HG21	1:A:350:LYS:HZ2	1.48	0.78
1:B:61:ASN:ND2	1:B:64:ASP:H	1.82	0.78
1:A:412:SER:HB3	1:A:430:ILE:HD12	1.68	0.76
1:B:210:ARG:O	1:B:214:GLU:HG2	1.85	0.74
1:B:175:THR:H	1:B:178:GLN:HE21	1.31	0.74
1:A:61:ASN:HD22	1:A:61:ASN:C	1.93	0.74
1:A:61:ASN:HD21	1:A:64:ASP:H	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:VAL:CG1	1:A:325:VAL:HG21	2.18	0.73
1:B:35:TRP:HE1	1:B:41:GLN:HE22	1.36	0.73
1:A:295:PRO:HG2	1:A:304:PHE:CD1	2.24	0.73
1:B:49:LEU:HD22	1:B:160:ALA:HB2	1.71	0.72
1:A:210:ARG:O	1:A:214:GLU:HG2	1.89	0.72
1:B:61:ASN:C	1:B:61:ASN:HD22	1.97	0.72
1:A:96:ILE:HG21	1:A:102:ILE:HD11	1.70	0.71
1:A:49:LEU:HD22	1:A:160:ALA:HB2	1.72	0.71
1:B:314:VAL:CG1	1:B:325:VAL:HG21	2.20	0.71
1:A:35:TRP:HE1	1:A:41:GLN:HE22	1.38	0.71
1:A:298:ASN:C	1:A:298:ASN:HD22	1.98	0.70
1:B:295:PRO:HG2	1:B:304:PHE:CD1	2.27	0.70
1:B:290:ARG:HD2	9:B:1001:HOH:O	1.92	0.70
1:B:96:ILE:HG21	1:B:102:ILE:HD11	1.73	0.69
1:B:469:LYS:H	1:B:469:LYS:CE	2.02	0.69
1:A:98:PRO:O	1:A:99:ASP:HB2	1.93	0.69
1:A:201:HIS:H	1:A:204:HIS:HD2	1.38	0.69
1:B:98:PRO:O	1:B:99:ASP:HB2	1.91	0.69
1:A:175:THR:H	1:A:178:GLN:NE2	1.90	0.69
1:B:201:HIS:H	1:B:204:HIS:HD2	1.41	0.68
1:B:314:VAL:HG11	1:B:325:VAL:HG21	1.76	0.67
1:A:362:ARG:HB2	1:A:362:ARG:CZ	2.23	0.67
1:A:366:ARG:HH21	1:A:366:ARG:HG2	1.58	0.67
1:A:352:ARG:HB3	1:A:352:ARG:NH2	2.10	0.67
1:B:362:ARG:HB2	1:B:362:ARG:CZ	2.22	0.67
1:A:329:ARG:H	1:A:329:ARG:CD	1.92	0.67
1:A:352:ARG:HA	9:A:649:HOH:O	1.95	0.66
1:B:298:ASN:C	1:B:298:ASN:HD22	2.03	0.66
1:B:166:HIS:HD2	9:B:646:HOH:O	1.78	0.66
1:B:61:ASN:HD21	1:B:64:ASP:H	1.44	0.66
1:B:366:ARG:HG2	1:B:366:ARG:HH21	1.60	0.66
1:A:67:SER:O	1:A:71:ASP:HB2	1.95	0.66
1:A:58:GLY:HA2	1:A:158:LEU:CD2	2.23	0.66
1:B:175:THR:H	1:B:178:GLN:NE2	1.93	0.65
1:B:247:LYS:HE3	9:B:1031:HOH:O	1.97	0.65
1:A:124:ASN:HD21	1:A:126:THR:HB	1.62	0.65
1:B:67:SER:O	1:B:71:ASP:HB2	1.96	0.65
1:B:352:ARG:NH2	1:B:352:ARG:HB3	2.11	0.65
1:A:314:VAL:HG11	1:A:325:VAL:HG21	1.79	0.65
1:B:201:HIS:H	1:B:204:HIS:CD2	2.15	0.64
1:A:243:GLN:O	1:A:246:ILE:HG22	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LYS:H	1:A:469:LYS:CE	2.09	0.63
1:B:243:GLN:O	1:B:246:ILE:HG22	1.99	0.62
1:A:201:HIS:H	1:A:204:HIS:CD2	2.17	0.62
1:B:363:ARG:O	1:B:367:VAL:HG13	2.00	0.62
1:A:348:THR:C	1:A:350:LYS:H	2.08	0.62
1:A:166:HIS:HD2	9:A:705:HOH:O	1.83	0.61
1:A:169:TYR:N	1:A:170:PRO:HD3	2.15	0.61
1:B:435:ASN:HD21	1:B:460:GLU:HB2	1.66	0.61
1:A:363:ARG:O	1:A:367:VAL:HG13	2.01	0.61
1:B:348:THR:C	1:B:350:LYS:H	2.08	0.61
1:A:351:THR:HG21	9:A:1192:HOH:O	2.00	0.60
1:A:335:PRO:HG3	1:A:354:LEU:HD12	1.83	0.60
1:B:298:ASN:HD21	1:B:302:VAL:HG13	1.65	0.60
1:B:124:ASN:HD21	1:B:126:THR:HB	1.66	0.60
1:B:180:ARG:O	1:B:184:GLN:HG3	2.02	0.60
1:B:362:ARG:CB	1:B:362:ARG:HH11	2.15	0.60
1:A:2:PRO:HD2	9:A:1105:HOH:O	2.01	0.60
1:B:207:LEU:C	1:B:207:LEU:HD23	2.27	0.60
1:A:20:LYS:HB3	8:A:550:ACY:H2	1.84	0.59
1:A:364:ARG:HA	1:A:367:VAL:HG22	1.84	0.59
1:B:115:LEU:HD23	1:B:158:LEU:HD13	1.85	0.59
1:B:188:TRP:CE2	1:B:218:LYS:HG3	2.37	0.59
1:A:352:ARG:CB	1:A:352:ARG:HH21	2.15	0.59
1:B:335:PRO:HD2	1:B:352:ARG:O	2.01	0.59
1:B:364:ARG:HA	1:B:367:VAL:HG22	1.84	0.59
1:B:382:LYS:HD3	9:B:770:HOH:O	2.02	0.59
1:B:172:LEU:HD12	1:B:172:LEU:N	2.17	0.59
1:B:362:ARG:NH1	1:B:362:ARG:CB	2.63	0.59
1:B:240:ARG:HD2	9:B:878:HOH:O	2.03	0.59
1:A:46:GLU:HB2	1:A:164:PRO:HD2	1.84	0.58
1:A:362:ARG:HH11	1:A:362:ARG:CB	2.16	0.58
1:A:362:ARG:NH1	1:A:362:ARG:CB	2.64	0.58
1:A:385:ARG:HA	9:A:760:HOH:O	2.02	0.58
1:A:435:ASN:HD21	1:A:460:GLU:HB2	1.69	0.58
1:B:46:GLU:HB2	1:B:164:PRO:HD2	1.85	0.58
1:A:180:ARG:O	1:A:184:GLN:HG3	2.04	0.58
1:A:362:ARG:HB2	1:A:362:ARG:HH11	1.64	0.58
1:B:169:TYR:N	1:B:170:PRO:HD3	2.19	0.57
1:B:352:ARG:CB	1:B:352:ARG:HH21	2.16	0.57
1:B:101:ARG:NH1	1:B:114:ILE:HG21	2.20	0.57
1:B:335:PRO:HG3	1:B:354:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ILE:HG23	1:A:360:GLU:HG3	1.86	0.56
1:A:363:ARG:O	1:A:367:VAL:HG22	2.05	0.56
1:A:329:ARG:HD3	1:A:342:PRO:HB3	1.87	0.56
1:A:438:GLU:HG2	9:A:1100:HOH:O	2.03	0.56
1:B:298:ASN:ND2	1:B:302:VAL:HG13	2.19	0.56
1:A:335:PRO:HD2	1:A:352:ARG:O	2.05	0.56
1:B:329:ARG:HG2	1:B:344:ASP:HB3	1.88	0.56
1:A:207:LEU:C	1:A:207:LEU:HD23	2.30	0.56
1:A:115:LEU:HD23	1:A:158:LEU:HD13	1.88	0.55
1:A:172:LEU:N	1:A:172:LEU:HD12	2.20	0.55
1:B:58:GLY:HA2	1:B:158:LEU:CD2	2.33	0.55
1:A:202:ARG:HH21	1:A:202:ARG:HG3	1.71	0.55
1:A:357:SER:HB2	9:A:755:HOH:O	2.06	0.55
1:A:298:ASN:HD21	1:A:302:VAL:HG13	1.71	0.55
1:B:20:LYS:HB3	8:B:560:ACY:H2	1.89	0.55
1:A:298:ASN:C	1:A:298:ASN:ND2	2.65	0.54
1:B:274:HIS:ND1	1:B:292:HIS:HE1	2.05	0.54
1:A:366:ARG:HG3	1:A:394:GLN:HE22	1.71	0.54
1:B:356:ILE:HG23	1:B:360:GLU:HG3	1.89	0.54
1:A:38:THR:H	1:A:41:GLN:NE2	2.05	0.53
1:B:178:GLN:O	1:B:182:GLU:HG2	2.07	0.53
1:B:348:THR:HG21	1:B:350:LYS:NZ	2.20	0.53
1:A:329:ARG:HG2	1:A:344:ASP:HB3	1.89	0.53
1:A:347:ASP:CG	1:A:348:THR:H	2.15	0.53
1:B:329:ARG:HD3	1:B:342:PRO:HB3	1.91	0.53
1:A:346:ILE:HG13	1:A:347:ASP:N	2.24	0.53
1:B:38:THR:H	1:B:41:GLN:NE2	2.06	0.53
1:B:352:ARG:HB3	1:B:352:ARG:HH21	1.71	0.53
1:A:437:THR:HG22	1:A:463:LYS:HD3	1.91	0.53
1:A:289:GLY:HA3	6:A:635:ADX:N3	2.24	0.53
1:A:298:ASN:ND2	1:A:302:VAL:HG13	2.24	0.53
1:A:352:ARG:HB3	1:A:352:ARG:HH21	1.71	0.53
1:A:124:ASN:HD22	1:A:124:ASN:C	2.17	0.52
1:A:462:ASP:OD1	1:A:463:LYS:HG3	2.09	0.52
1:A:274:HIS:ND1	1:A:292:HIS:HE1	2.07	0.52
1:B:362:ARG:HB2	1:B:362:ARG:HH11	1.65	0.52
1:B:124:ASN:C	1:B:124:ASN:HD22	2.17	0.52
1:A:343:ILE:HD12	1:A:346:ILE:HD11	1.90	0.52
1:A:400:LEU:HG	1:A:456:PRO:HA	1.92	0.52
1:A:22:GLU:OE2	1:A:22:GLU:N	2.36	0.52
1:B:61:ASN:HA	1:B:155:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASN:HA	1:A:155:GLY:HA3	1.92	0.51
1:B:309:ASP:HB3	9:B:704:HOH:O	2.11	0.51
1:B:363:ARG:O	1:B:367:VAL:HG22	2.10	0.51
1:B:347:ASP:CG	1:B:348:THR:H	2.18	0.51
1:B:343:ILE:HD12	1:B:346:ILE:HD11	1.92	0.51
1:B:437:THR:HG22	1:B:463:LYS:HD3	1.92	0.50
1:A:391:ARG:N	1:A:392:PRO:HD2	2.26	0.50
1:B:366:ARG:HG3	1:B:394:GLN:HE22	1.77	0.50
1:A:348:THR:HG21	1:A:350:LYS:NZ	2.22	0.50
1:A:101:ARG:NH1	1:A:114:ILE:HG21	2.25	0.50
1:B:106:GLN:NE2	1:B:165:GLN:H	1.94	0.50
1:A:173:ARG:HG2	1:A:173:ARG:HH21	1.77	0.50
1:A:61:ASN:ND2	1:A:61:ASN:C	2.67	0.49
6:A:635:ADX:N7	7:A:637:POP:O6	2.45	0.49
1:B:346:ILE:HG13	1:B:347:ASP:N	2.27	0.49
1:B:510:VAL:HA	9:B:841:HOH:O	2.11	0.49
1:B:469:LYS:H	1:B:469:LYS:CD	2.25	0.49
1:A:285:HIS:HA	1:A:324:GLU:O	2.12	0.49
1:B:123:PRO:HG3	1:B:153:TYR:CE1	2.47	0.49
1:A:347:ASP:CG	1:A:348:THR:N	2.68	0.49
1:A:12:LEU:HD22	1:A:15:ARG:CZ	2.43	0.49
1:A:346:ILE:HG13	1:A:347:ASP:H	1.78	0.49
1:A:358:GLY:N	9:A:755:HOH:O	2.39	0.49
1:B:330:MET:HE2	9:B:1001:HOH:O	2.12	0.49
1:A:469:LYS:H	1:A:469:LYS:CD	2.25	0.49
1:B:124:ASN:HD22	1:B:127:ILE:H	1.60	0.49
1:A:178:GLN:O	1:A:182:GLU:HG2	2.12	0.48
1:B:171:GLY:O	1:B:174:LYS:HE2	2.13	0.48
1:B:401:GLY:HA3	1:B:476:ASP:OD1	2.12	0.48
1:A:345:GLN:O	1:A:346:ILE:HG23	2.12	0.48
1:A:401:GLY:HA3	1:A:476:ASP:OD1	2.13	0.48
1:A:29:SER:O	1:A:32:ILE:HG22	2.14	0.48
1:A:292:HIS:CD2	6:A:635:ADX:O3'	2.67	0.48
1:A:346:ILE:CG1	1:A:347:ASP:H	2.26	0.48
1:B:179:LEU:O	1:B:182:GLU:HB2	2.13	0.48
1:B:462:ASP:OD1	1:B:463:LYS:HG3	2.13	0.48
1:B:2:PRO:HD2	9:B:658:HOH:O	2.13	0.48
1:B:391:ARG:N	1:B:392:PRO:HD2	2.28	0.48
1:B:435:ASN:HD21	1:B:460:GLU:CB	2.27	0.48
1:B:12:LEU:HD22	1:B:15:ARG:CZ	2.43	0.48
1:B:438:GLU:HG2	9:B:949:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLU:OE2	1:B:22:GLU:N	2.30	0.47
1:A:461:ASP:HB3	9:A:851:HOH:O	2.13	0.47
1:B:61:ASN:ND2	1:B:61:ASN:C	2.69	0.47
1:B:347:ASP:CG	1:B:348:THR:N	2.70	0.47
1:A:188:TRP:CE2	1:A:218:LYS:HG3	2.48	0.47
1:B:202:ARG:HH21	1:B:202:ARG:HG3	1.79	0.47
1:B:476:ASP:HB3	1:B:481:ALA:HB2	1.97	0.47
1:A:43:CYS:CB	1:A:262:ALA:HB2	2.45	0.47
1:A:173:ARG:HG2	1:A:173:ARG:NH2	2.30	0.47
1:B:223:PRO:HD2	1:B:257:SER:O	2.14	0.47
1:A:435:ASN:HD21	1:A:460:GLU:CB	2.28	0.47
1:B:107:ASP:O	1:B:108:ASP:C	2.58	0.47
1:B:298:ASN:HD21	1:B:302:VAL:CG1	2.28	0.47
1:B:43:CYS:CB	1:B:262:ALA:HB2	2.45	0.47
1:B:133:PHE:O	1:B:134:ARG:HB2	2.13	0.47
1:B:285:HIS:HA	1:B:324:GLU:O	2.14	0.47
1:A:202:ARG:HG2	1:A:377:TYR:CE1	2.50	0.47
1:B:297:LYS:HD3	1:B:301:GLY:O	2.14	0.47
1:B:298:ASN:C	1:B:298:ASN:ND2	2.69	0.47
1:A:297:LYS:HD3	1:A:301:GLY:O	2.15	0.46
1:B:35:TRP:HE1	1:B:41:GLN:NE2	2.09	0.46
1:A:492:ILE:O	1:A:496:VAL:HG23	2.15	0.46
1:B:400:LEU:HG	1:B:456:PRO:HA	1.97	0.46
1:B:290:ARG:HG3	1:B:308:TYR:CZ	2.51	0.46
1:B:29:SER:O	1:B:32:ILE:HG22	2.16	0.46
1:B:184:GLN:C	1:B:186:ARG:N	2.73	0.46
1:B:335:PRO:HG3	1:B:354:LEU:CD1	2.46	0.46
1:B:346:ILE:CG1	1:B:347:ASP:H	2.29	0.46
1:A:35:TRP:HE1	1:A:41:GLN:NE2	2.10	0.46
1:A:124:ASN:ND2	1:A:127:ILE:H	2.14	0.46
1:A:335:PRO:HG3	1:A:354:LEU:CD1	2.45	0.46
1:A:339:ARG:HH22	1:A:341:ALA:HB2	1.80	0.46
1:B:106:GLN:HE21	1:B:112:ILE:HD11	1.81	0.46
1:A:133:PHE:O	1:A:134:ARG:HB2	2.15	0.46
1:A:172:LEU:HB3	1:A:258:LEU:HG	1.98	0.46
1:A:230:PRO:HD2	9:A:873:HOH:O	2.16	0.46
1:B:173:ARG:HG2	1:B:173:ARG:HH21	1.81	0.46
1:A:358:GLY:O	1:A:361:LEU:HB3	2.15	0.46
1:A:363:ARG:HG2	1:A:363:ARG:HH21	1.80	0.45
1:B:76:ASP:C	1:B:76:ASP:OD2	2.60	0.45
1:A:76:ASP:OD2	1:A:76:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:HB3	1:B:258:LEU:HG	1.99	0.45
1:B:123:PRO:HG3	1:B:153:TYR:CZ	2.51	0.45
1:A:95:GLN:HB3	9:A:756:HOH:O	2.15	0.45
1:A:356:ILE:HG23	1:A:360:GLU:CG	2.47	0.45
1:B:96:ILE:HG13	1:B:120:VAL:HG21	1.99	0.45
1:B:124:ASN:ND2	1:B:127:ILE:H	2.15	0.45
1:B:347:ASP:C	1:B:349:THR:N	2.74	0.45
1:A:329:ARG:HD3	1:A:344:ASP:OD1	2.17	0.45
1:B:358:GLY:O	1:B:361:LEU:HB3	2.16	0.45
1:A:336:ASP:CG	1:A:352:ARG:HH22	2.25	0.45
1:A:352:ARG:NH2	1:A:352:ARG:CB	2.77	0.45
1:B:466:VAL:O	1:B:466:VAL:HG12	2.15	0.45
1:A:458:GLN:HB3	9:A:1190:HOH:O	2.17	0.45
1:B:491:PRO:HG2	1:B:494:HIS:CG	2.52	0.45
1:A:42:LEU:HD11	1:A:106:GLN:HG3	2.00	0.44
1:B:418:THR:O	1:B:421:GLN:HG2	2.17	0.44
1:A:261:LEU:HG	1:A:262:ALA:N	2.32	0.44
1:B:492:ILE:O	1:B:496:VAL:HG23	2.18	0.44
1:A:97:LYS:HD2	9:A:1217:HOH:O	2.16	0.44
1:B:268:ASP:HA	1:B:310:ALA:HA	2.00	0.44
1:A:366:ARG:HH21	1:A:366:ARG:CG	2.28	0.44
1:B:434:ASN:O	1:B:436:LYS:HG3	2.17	0.44
1:A:171:GLY:O	1:A:174:LYS:HE2	2.17	0.44
1:A:494:HIS:HD1	8:A:552:ACY:C	2.30	0.44
1:B:172:LEU:N	1:B:172:LEU:CD1	2.81	0.44
1:B:202:ARG:HG2	1:B:377:TYR:CE1	2.52	0.44
1:B:261:LEU:HG	1:B:262:ALA:N	2.33	0.44
1:B:409:GLU:CD	1:B:409:GLU:H	2.25	0.44
1:A:403:SER:O	1:A:488:ALA:HB1	2.18	0.44
1:B:346:ILE:HG13	1:B:347:ASP:H	1.82	0.44
6:A:635:ADX:H5 ⁺	6:A:635:ADX:SB	2.58	0.44
1:B:313:LEU:HD22	1:B:317:TYR:CE1	2.53	0.44
1:B:348:THR:C	1:B:350:LYS:N	2.74	0.44
1:B:403:SER:O	1:B:488:ALA:HB1	2.18	0.44
1:A:298:ASN:HD21	1:A:302:VAL:CG1	2.31	0.44
1:B:366:ARG:HH21	1:B:366:ARG:CG	2.29	0.44
1:A:435:ASN:ND2	1:A:460:GLU:HG2	2.33	0.43
1:A:476:ASP:HB3	1:A:481:ALA:HB2	2.00	0.43
1:A:491:PRO:HG2	1:A:494:HIS:CG	2.53	0.43
1:B:115:LEU:HD13	1:B:115:LEU:C	2.43	0.43
1:B:347:ASP:C	1:B:349:THR:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ILE:HG23	1:B:360:GLU:CG	2.48	0.43
1:B:459:TRP:NE1	1:B:464:ASP:HA	2.33	0.43
1:A:385:ARG:HH21	1:A:385:ARG:HG2	1.82	0.43
1:B:112:ILE:O	1:B:161:ILE:HB	2.19	0.43
1:B:186:ARG:NH1	8:B:564:ACY:O	2.52	0.43
1:A:348:THR:C	1:A:350:LYS:N	2.74	0.43
1:A:418:THR:O	1:A:421:GLN:CG	2.67	0.43
1:B:325:VAL:O	1:B:327:PRO:HD3	2.18	0.43
1:A:192:VAL:HA	1:A:285:HIS:HB2	2.01	0.43
1:A:329:ARG:O	1:A:330:MET:C	2.60	0.43
1:B:173:ARG:HG2	1:B:173:ARG:NH2	2.33	0.43
1:B:266:SER:O	1:B:267:GLY:C	2.61	0.43
1:A:409:GLU:H	1:A:409:GLU:CD	2.27	0.43
1:B:42:LEU:HD11	1:B:106:GLN:HG3	2.01	0.43
1:B:316:SER:HB3	9:B:1131:HOH:O	2.18	0.43
1:B:339:ARG:HH22	1:B:341:ALA:HB2	1.84	0.43
1:A:123:PRO:HG3	1:A:153:TYR:CE1	2.54	0.43
1:B:219:VAL:O	1:B:254:ALA:HA	2.19	0.43
1:A:329:ARG:HG2	1:A:344:ASP:CG	2.44	0.43
1:A:172:LEU:N	1:A:172:LEU:CD1	2.82	0.42
1:B:60:LEU:HA	9:B:905:HOH:O	2.18	0.42
1:A:169:TYR:N	1:A:170:PRO:CD	2.83	0.42
1:A:347:ASP:C	1:A:349:THR:N	2.77	0.42
1:B:359:THR:HG23	1:B:362:ARG:HH21	1.85	0.42
1:B:393:LYS:HA	9:B:999:HOH:O	2.19	0.42
1:A:42:LEU:O	1:A:45:ILE:HG22	2.20	0.42
1:B:366:ARG:HD3	9:B:1029:HOH:O	2.20	0.42
1:A:136:ASP:HA	1:A:137:PRO:HD2	1.89	0.42
1:A:268:ASP:HA	1:A:310:ALA:HA	2.02	0.42
1:A:390:PRO:C	1:A:392:PRO:HD2	2.45	0.42
1:B:124:ASN:C	1:B:124:ASN:ND2	2.78	0.42
1:A:290:ARG:NH2	1:A:307:PRO:HB3	2.34	0.42
1:A:390:PRO:HB2	1:A:392:PRO:HD2	2.02	0.42
1:B:192:VAL:HA	1:B:285:HIS:HB2	2.01	0.42
1:B:207:LEU:C	1:B:207:LEU:CD2	2.93	0.42
1:B:455:ILE:HA	1:B:456:PRO:HD2	1.86	0.42
1:A:16:ASP:OD1	1:A:159:GLU:HA	2.19	0.41
1:A:107:ASP:O	1:A:108:ASP:C	2.63	0.41
1:A:112:ILE:O	1:A:161:ILE:HB	2.20	0.41
1:A:330:MET:HB3	1:A:343:ILE:HG21	2.02	0.41
1:B:166:HIS:CD2	9:B:711:HOH:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:O	1:A:187:GLN:HB2	2.19	0.41
1:B:313:LEU:HD23	1:B:313:LEU:HA	1.89	0.41
1:A:212:ALA:HB2	1:A:219:VAL:CG2	2.51	0.41
1:A:272:VAL:HG21	1:A:313:LEU:HD13	2.02	0.41
1:A:347:ASP:C	1:A:349:THR:H	2.28	0.41
1:B:378:PRO:HG2	1:B:379:GLU:HG3	2.02	0.41
1:B:458:GLN:HE21	1:B:458:GLN:HB3	1.58	0.41
1:B:212:ALA:HB2	1:B:219:VAL:CG2	2.50	0.41
1:B:345:GLN:O	1:B:346:ILE:HG23	2.21	0.41
1:A:261:LEU:HD11	1:A:273:TRP:CH2	2.56	0.41
1:A:96:ILE:HG13	1:A:120:VAL:HG21	2.02	0.41
1:A:46:GLU:OE2	1:A:166:HIS:HE1	2.04	0.41
1:A:123:PRO:HG3	1:A:153:TYR:CZ	2.56	0.41
1:A:266:SER:O	1:A:267:GLY:C	2.63	0.41
1:A:292:HIS:HD2	6:A:635:ADX:O3'	2.03	0.41
1:B:40:ARG:HG3	1:B:262:ALA:HB1	2.03	0.41
1:B:186:ARG:O	1:B:187:GLN:HB2	2.20	0.41
1:A:90:GLU:HG3	9:A:747:HOH:O	2.21	0.41
1:A:295:PRO:HG2	1:A:304:PHE:CG	2.56	0.41
1:B:184:GLN:O	1:B:185:SER:C	2.64	0.41
1:B:188:TRP:CD2	1:B:218:LYS:HG3	2.56	0.41
1:A:179:LEU:O	1:A:182:GLU:HB2	2.21	0.40
1:B:46:GLU:OE2	1:B:166:HIS:HE1	2.04	0.40
1:B:329:ARG:HG2	1:B:344:ASP:CG	2.46	0.40
1:A:26:GLU:OE1	1:A:101:ARG:NE	2.39	0.40
1:A:124:ASN:ND2	1:A:127:ILE:HG13	2.36	0.40
1:B:82:ILE:HG13	1:B:273:TRP:CE3	2.56	0.40
1:A:366:ARG:HG2	1:A:366:ARG:NH2	2.32	0.40
1:B:476:ASP:O	1:B:484:GLN:HA	2.21	0.40
1:B:348:THR:O	1:B:349:THR:HB	2.22	0.40
1:A:244:GLU:HG3	1:A:379:GLU:OE2	2.22	0.40
1:A:396:PHE:CD1	1:A:396:PHE:C	2.99	0.40
1:B:391:ARG:HD3	1:B:391:ARG:HA	1.86	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:515:CD:CD	2:B:533:CD:CD[2_765]	1.19	1.01

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	508/511 (99%)	475 (94%)	28 (6%)	5 (1%)	12	38
1	B	508/511 (99%)	470 (92%)	36 (7%)	2 (0%)	30	60
All	All	1016/1022 (99%)	945 (93%)	64 (6%)	7 (1%)	18	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	ILE
1	B	346	ILE
1	A	109	GLU
1	A	359	THR
1	B	359	THR
1	A	267	GLY
1	A	335	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/446 (100%)	426 (96%)	19 (4%)	26	60
1	B	445/446 (100%)	426 (96%)	19 (4%)	26	60
All	All	890/892 (100%)	852 (96%)	38 (4%)	26	60

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	24	LEU
1	A	31	ASP
1	A	61	ASN
1	A	124	ASN
1	A	158	LEU
1	A	179	LEU
1	A	202	ARG
1	A	206	GLU
1	A	216	ASN
1	A	298	ASN
1	A	302	VAL
1	A	313	LEU
1	A	329	ARG
1	A	379	GLU
1	A	405	THR
1	A	435	ASN
1	A	469	LYS
1	A	474	LEU
1	B	18	LEU
1	B	24	LEU
1	B	31	ASP
1	B	61	ASN
1	B	124	ASN
1	B	158	LEU
1	B	179	LEU
1	B	202	ARG
1	B	206	GLU
1	B	216	ASN
1	B	298	ASN
1	B	302	VAL
1	B	313	LEU
1	B	329	ARG
1	B	379	GLU
1	B	405	THR
1	B	435	ASN
1	B	469	LYS
1	B	474	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN

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Mol	Chain	Res	Type
1	A	21	ASN
1	A	28	GLN
1	A	41	GLN
1	A	61	ASN
1	A	63	ASN
1	A	94	ASN
1	A	95	GLN
1	A	106	GLN
1	A	118	GLN
1	A	124	ASN
1	A	147	ASN
1	A	166	HIS
1	A	178	GLN
1	A	184	GLN
1	A	198	ASN
1	A	204	HIS
1	A	243	GLN
1	A	292	HIS
1	A	298	ASN
1	A	388	ASN
1	A	434	ASN
1	A	435	ASN
1	A	471	ASN
1	A	484	GLN
1	A	506	ASN
1	B	10	GLN
1	B	21	ASN
1	B	41	GLN
1	B	61	ASN
1	B	63	ASN
1	B	94	ASN
1	B	106	GLN
1	B	118	GLN
1	B	124	ASN
1	B	147	ASN
1	B	166	HIS
1	B	178	GLN
1	B	184	GLN
1	B	198	ASN
1	B	204	HIS
1	B	236	HIS
1	B	243	GLN

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Mol	Chain	Res	Type
1	B	292	HIS
1	B	298	ASN
1	B	434	ASN
1	B	435	ASN
1	B	471	ASN
1	B	484	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 50 ligands modelled in this entry, 31 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	ACY	A	554	2	3,3,3	1.65	0	3,3,3	1.21	0
6	ADX	A	635	-	29,29,29	1.60	5 (17%)	42,45,45	2.06	9 (21%)
8	ACY	B	560	2	3,3,3	1.32	0	3,3,3	1.33	0
8	ACY	B	565	2	3,3,3	1.47	0	3,3,3	1.23	0
8	ACY	B	566	2	3,3,3	1.54	0	3,3,3	1.24	0
8	ACY	A	553	-	3,3,3	1.57	0	3,3,3	1.16	0
8	ACY	A	550	2	3,3,3	1.46	0	3,3,3	1.26	0
8	ACY	A	567	2	3,3,3	1.52	0	3,3,3	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ACY	A	556	2	3,3,3	1.41	0	3,3,3	1.33	0
8	ACY	B	561	2	3,3,3	1.54	0	3,3,3	1.24	0
6	ADX	B	636	-	29,29,29	1.54	5 (17%)	42,45,45	2.04	9 (21%)
8	ACY	A	552	-	3,3,3	1.59	0	3,3,3	1.19	0
7	POP	B	638	-	6,8,8	1.46	0	12,13,13	1.41	3 (25%)
8	ACY	A	555	2	3,3,3	1.48	0	3,3,3	1.21	0
8	ACY	B	564	2	3,3,3	1.57	0	3,3,3	1.32	0
7	POP	A	637	-	6,8,8	1.50	0	12,13,13	1.37	2 (16%)
8	ACY	B	562	-	3,3,3	1.44	0	3,3,3	1.28	0
8	ACY	A	551	2	3,3,3	1.48	0	3,3,3	1.29	0
8	ACY	B	563	-	3,3,3	1.55	0	3,3,3	1.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADX	B	636	-	-	2/10/32/32	0/3/3/3
6	ADX	A	635	-	-	2/10/32/32	0/3/3/3
7	POP	A	637	-	-	2/6/6/6	-
7	POP	B	638	-	-	5/6/6/6	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	635	ADX	C5-N7	-4.65	1.30	1.39
6	B	636	ADX	O2B-SB	4.32	1.64	1.45
6	B	636	ADX	C5-N7	-3.96	1.31	1.39
6	A	635	ADX	O2B-SB	3.92	1.62	1.45
6	A	635	ADX	O3A-SB	-2.81	1.53	1.65
6	A	635	ADX	C4-N9	-2.69	1.32	1.37
6	B	636	ADX	C4-N9	-2.68	1.32	1.37
6	A	635	ADX	C8-N9	-2.66	1.33	1.37
6	B	636	ADX	O3A-SB	-2.32	1.55	1.65
6	B	636	ADX	C8-N9	-2.22	1.33	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	636	ADX	N3-C2-N1	-6.46	118.80	128.58
6	A	635	ADX	N3-C2-N1	-6.46	118.81	128.58
6	B	636	ADX	C5-C4-N3	-5.37	119.32	126.72
6	A	635	ADX	C5-C4-N3	-5.32	119.40	126.72
6	B	636	ADX	C2-N3-C4	4.59	123.05	111.83
6	A	635	ADX	C2-N3-C4	4.50	122.81	111.83
6	A	635	ADX	N3-C4-N9	3.99	133.95	127.17
6	B	636	ADX	N3-C4-N9	3.81	133.65	127.17
6	A	635	ADX	C5-N7-C8	3.62	109.14	103.45
6	B	636	ADX	C5-N7-C8	3.45	108.88	103.45
6	B	636	ADX	C4-C5-N7	-3.44	106.65	110.58
6	A	635	ADX	N9-C8-N7	-3.40	109.12	113.94
6	B	636	ADX	N9-C8-N7	-3.38	109.14	113.94
6	A	635	ADX	C4-C5-N7	-3.35	106.76	110.58
7	A	637	POP	O5-P2-O4	-2.75	100.13	110.83
7	B	638	POP	O5-P2-O4	-2.52	101.00	110.83
6	A	635	ADX	C4-N9-C8	2.47	108.33	105.74
6	B	636	ADX	C4-N9-C8	2.44	108.30	105.74
7	B	638	POP	O6-P2-O4	2.43	120.31	110.83
6	A	635	ADX	O3B-SB-O3A	2.41	111.17	106.02
7	A	637	POP	O6-P2-O4	2.33	119.92	110.83
7	B	638	POP	O6-P2-O	2.14	111.80	104.64
6	B	636	ADX	C6-C5-N7	2.07	136.09	132.09

There are no chirality outliers.

All (11) torsion outliers are listed below:

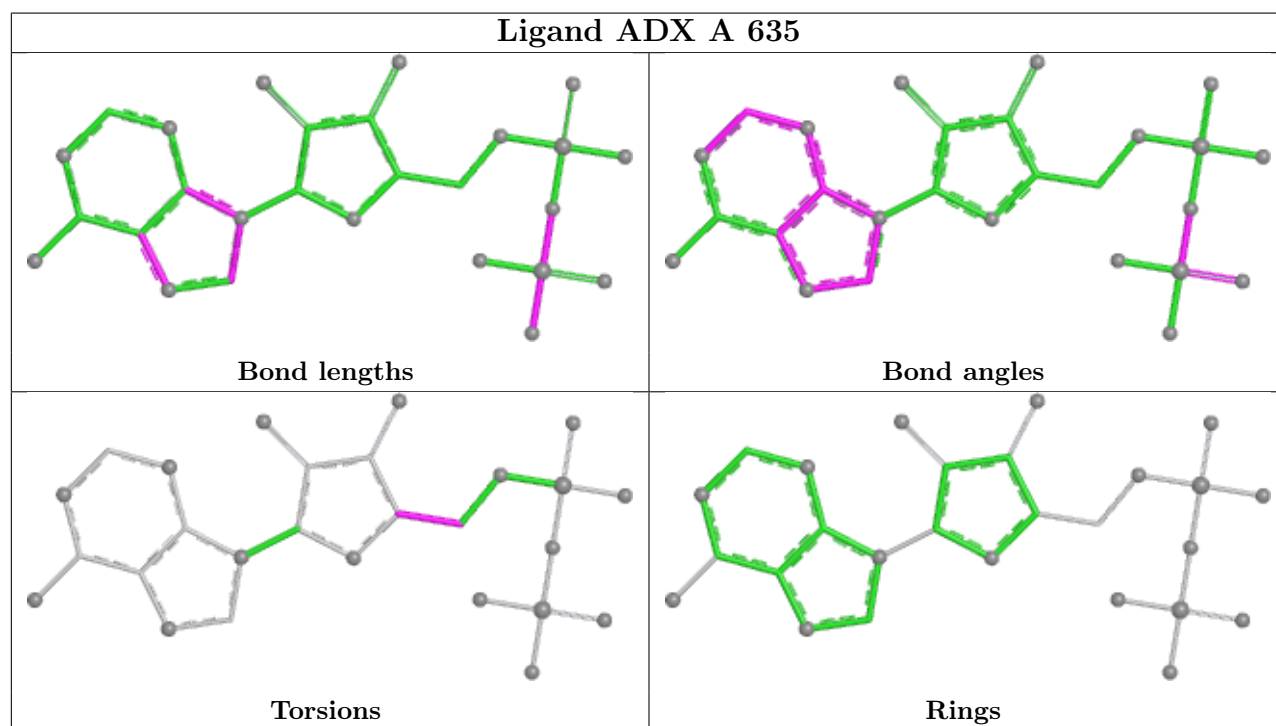
Mol	Chain	Res	Type	Atoms
7	A	637	POP	P2-O-P1-O2
7	A	637	POP	P2-O-P1-O3
7	B	638	POP	P2-O-P1-O3
7	B	638	POP	P1-O-P2-O6
6	B	636	ADX	O4'-C4'-C5'-O5'
6	A	635	ADX	O4'-C4'-C5'-O5'
6	B	636	ADX	C3'-C4'-C5'-O5'
7	B	638	POP	P1-O-P2-O4
7	B	638	POP	P2-O-P1-O2
7	B	638	POP	P1-O-P2-O5
6	A	635	ADX	C3'-C4'-C5'-O5'

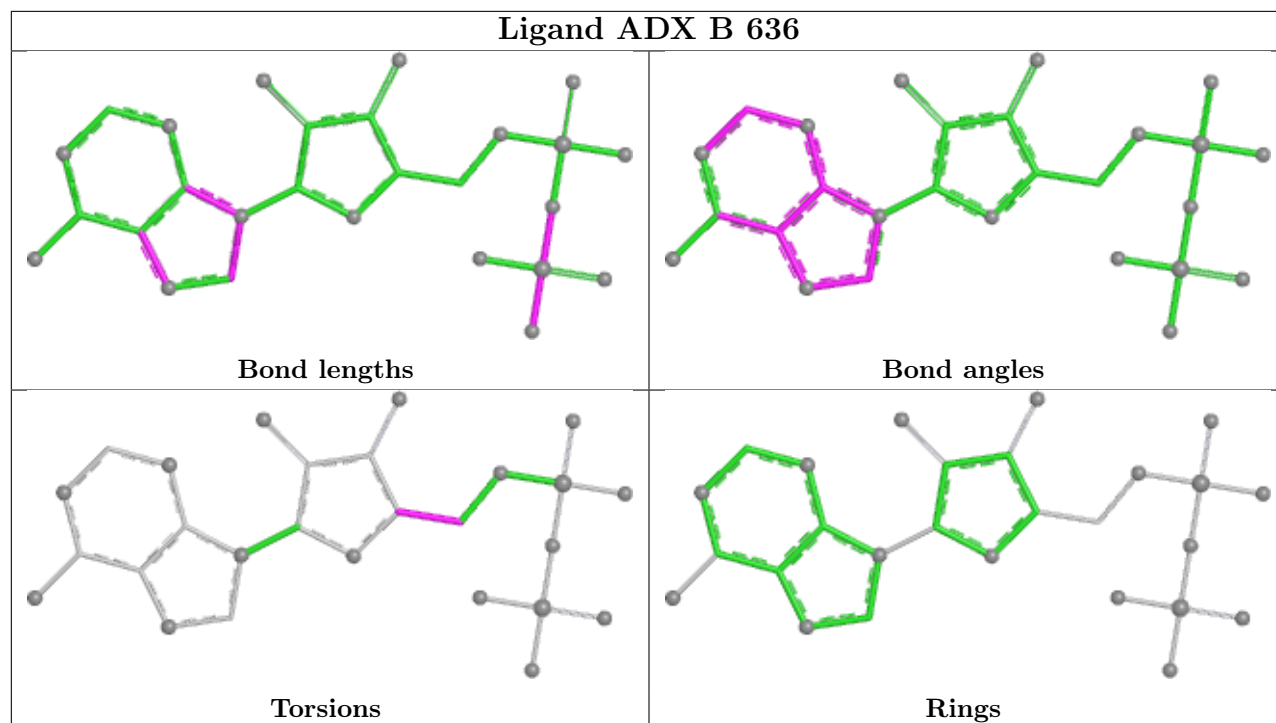
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	635	ADX	5	0
8	B	560	ACY	1	0
8	A	550	ACY	1	0
8	A	552	ACY	1	0
8	B	564	ACY	1	0
7	A	637	POP	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 [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

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	510/511 (99%)	-0.22	16 (3%) 51 41	15, 31, 72, 90	0
1	B	510/511 (99%)	-0.28	6 (1%) 76 68	14, 31, 72, 90	0
All	All	1020/1022 (99%)	-0.25	22 (2%) 62 52	14, 31, 72, 90	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	LEU	3.9
1	B	351	THR	3.6
1	B	355	ASN	3.4
1	A	351	THR	3.3
1	A	349	THR	3.1
1	A	354	LEU	2.8
1	A	355	ASN	2.6
1	A	356	ILE	2.5
1	A	346	ILE	2.4
1	A	334	LEU	2.4
1	A	362	ARG	2.3
1	B	370	GLU	2.3
1	A	405	THR	2.3
1	A	348	THR	2.3
1	A	359	THR	2.3
1	A	369	GLY	2.3
1	A	347	ASP	2.1
1	B	349	THR	2.1
1	B	358	GLY	2.1
1	A	338	ASP	2.1
1	A	367	VAL	2.0
1	B	364	ARG	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
8	ACY	B	562	4/4	0.70	0.25	63,64,65,65	0
8	ACY	A	552	4/4	0.79	0.20	53,54,55,55	0
8	ACY	A	553	4/4	0.86	0.15	34,36,36,36	0
3	CA	B	537	1/1	0.86	0.14	73,73,73,73	0
8	ACY	B	563	4/4	0.86	0.14	31,33,33,34	0
5	MG	B	539	1/1	0.87	0.20	70,70,70,70	0
7	POP	B	638	9/9	0.87	0.12	92,93,93,93	0
3	CA	A	519	1/1	0.89	0.10	63,63,63,63	0
4	NA	B	542	1/1	0.89	0.22	56,56,56,56	0
4	NA	B	540	1/1	0.90	0.12	30,30,30,30	0
4	NA	A	527	1/1	0.90	0.10	35,35,35,35	0
4	NA	B	536	1/1	0.93	0.25	42,42,42,42	0
4	NA	A	518	1/1	0.93	0.19	42,42,42,42	0
3	CA	A	520	1/1	0.93	0.09	45,45,45,45	0
7	POP	A	637	9/9	0.94	0.08	47,50,51,51	0
4	NA	B	544	1/1	0.94	0.13	29,29,29,29	0
8	ACY	A	551	4/4	0.95	0.13	35,36,37,38	0
8	ACY	A	555	4/4	0.95	0.12	46,47,48,49	0
5	MG	A	521	1/1	0.96	0.05	22,22,22,22	0
2	CD	A	513	1/1	0.96	0.08	127,127,127,127	0
2	CD	B	531	1/1	0.96	0.07	113,113,113,113	0
4	NA	A	523	1/1	0.96	0.04	35,35,35,35	0
3	CA	B	535	1/1	0.96	0.14	38,38,38,38	0
8	ACY	B	564	4/4	0.96	0.17	22,22,25,26	0
6	ADX	A	635	27/27	0.97	0.07	21,33,40,40	0
6	ADX	B	636	27/27	0.97	0.07	24,29,43,45	0
4	NA	A	525	1/1	0.97	0.11	6,6,6,6	0

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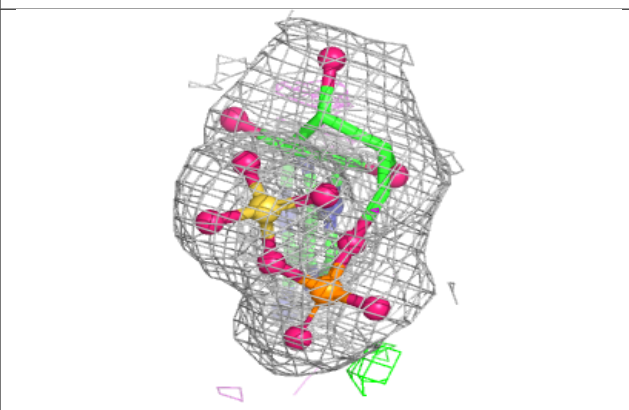
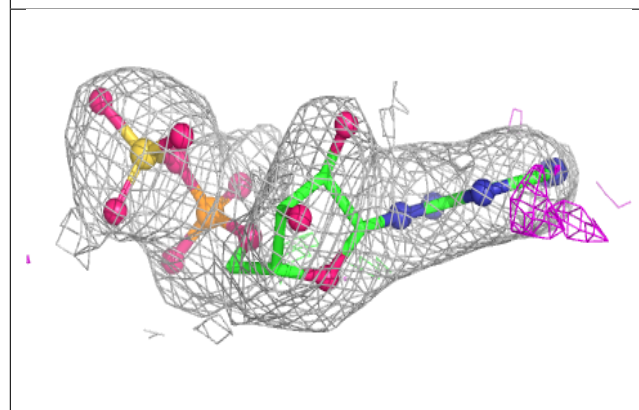
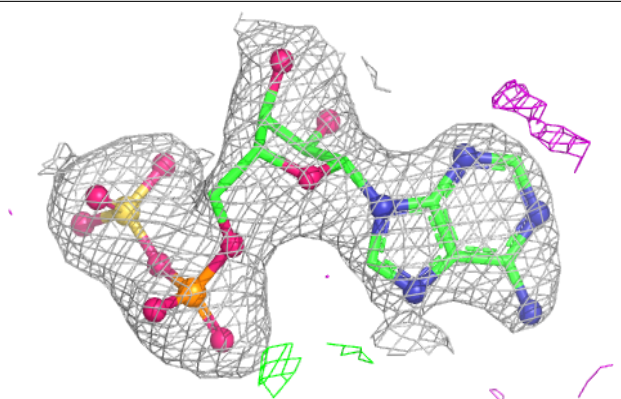
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ACY	A	567	4/4	0.97	0.08	21,24,25,27	0
4	NA	A	526	1/1	0.97	0.09	20,20,20,20	0
8	ACY	A	550	4/4	0.97	0.07	22,25,25,27	0
4	NA	A	522	1/1	0.97	0.09	19,19,19,19	0
8	ACY	B	566	4/4	0.97	0.08	22,24,25,25	0
8	ACY	B	561	4/4	0.98	0.11	29,32,32,33	0
8	ACY	A	554	4/4	0.98	0.08	19,21,22,23	0
4	NA	B	543	1/1	0.98	0.07	34,34,34,34	0
4	NA	B	541	1/1	0.98	0.05	20,20,20,20	0
8	ACY	B	565	4/4	0.98	0.12	73,74,74,74	0
8	ACY	B	560	4/4	0.98	0.06	29,30,30,31	0
3	CA	B	538	1/1	0.99	0.08	26,26,26,26	0
8	ACY	A	556	4/4	0.99	0.06	28,30,31,31	0
2	CD	B	532	1/1	0.99	0.02	40,40,40,40	0
3	CA	A	517	1/1	0.99	0.04	31,31,31,31	0
2	CD	A	524	1/1	0.99	0.03	56,56,56,56	0
2	CD	A	515	1/1	1.00	0.03	78,78,78,78	0
2	CD	B	533	1/1	1.00	0.02	47,47,47,47	0
2	CD	B	534	1/1	1.00	0.02	35,35,35,35	0
2	CD	A	516	1/1	1.00	0.01	43,43,43,43	0
2	CD	A	512	1/1	1.00	0.01	32,32,32,32	0
2	CD	B	530	1/1	1.00	0.01	38,38,38,38	0
2	CD	A	514	1/1	1.00	0.04	36,36,36,36	0

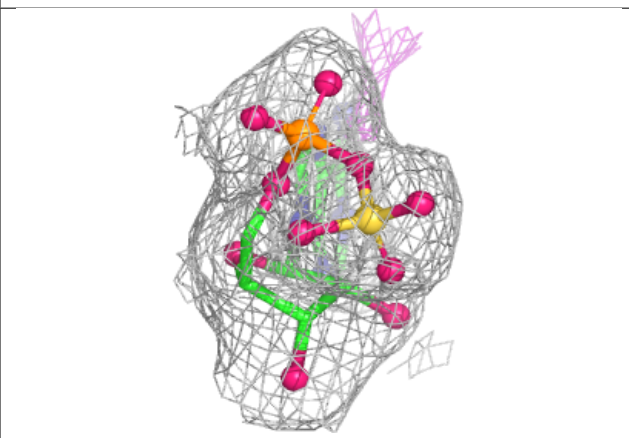
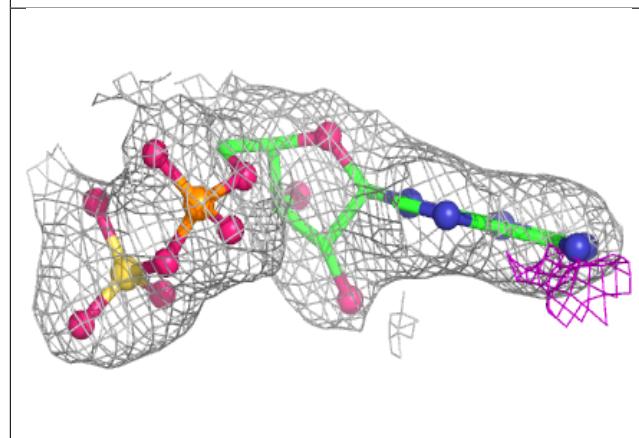
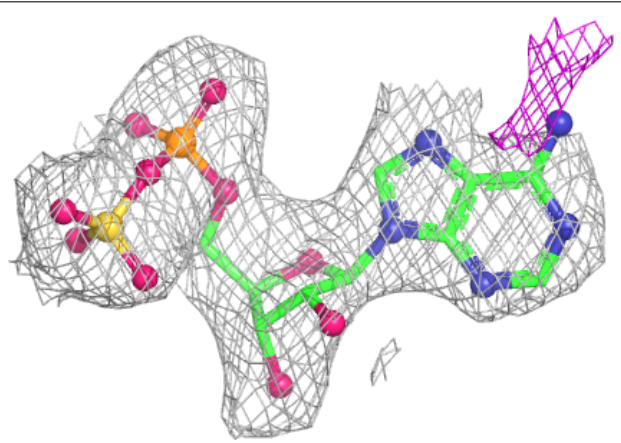
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADX A 635:

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

**Electron density around ADX B 636:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.