



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:28 AM UTC

PDB ID : 4MAF / pdb_00004maf
Title : Soybean ATP Sulfurylase
Authors : Herrmann, J.; Ravilious, G.E.; McKinney, S.E.; Westfall, C.S.; Lee, S.G.;
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Deposited on : 2013-08-16
Resolution : 2.48 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

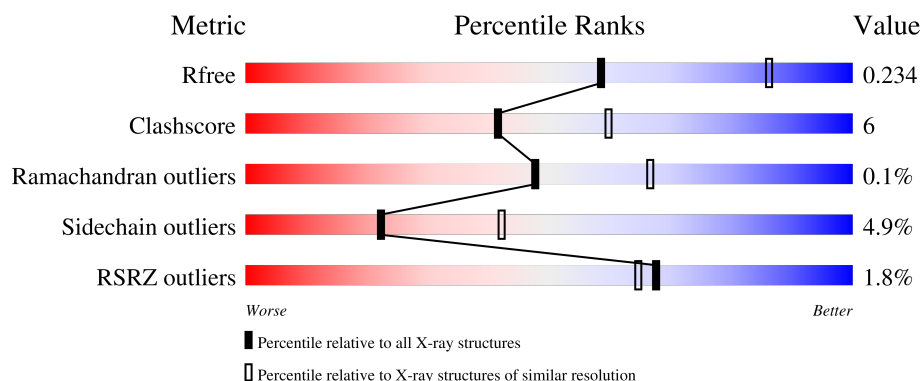
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	404	% 81% 16% .
1	B	404	85% 14% .
1	C	404	86% 13% .
1	D	404	% 82% 15% ..
1	E	404	2% 84% 14% .

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Mol	Chain	Length	Quality of chain
1	F	404	% 82% 16% ••
1	G	404	% 84% 14% •
1	H	404	7% 71% 21% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26495 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 ATP sulfurylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3197	2045	558	581	13			
1	B	404	Total	C	N	O	S	0	2	0
			3219	2059	560	587	13			
1	C	403	Total	C	N	O	S	0	0	0
			3205	2051	559	582	13			
1	D	401	Total	C	N	O	S	0	0	0
			3190	2040	557	580	13			
1	E	403	Total	C	N	O	S	0	0	0
			3205	2051	559	582	13			
1	F	401	Total	C	N	O	S	0	0	0
			3190	2040	557	580	13			
1	G	404	Total	C	N	O	S	0	0	0
			3211	2054	560	584	13			
1	H	381	Total	C	N	O	S	0	0	0
			3037	1948	528	550	11			

There are 24 discrepancies between the modelled and reference sequences:

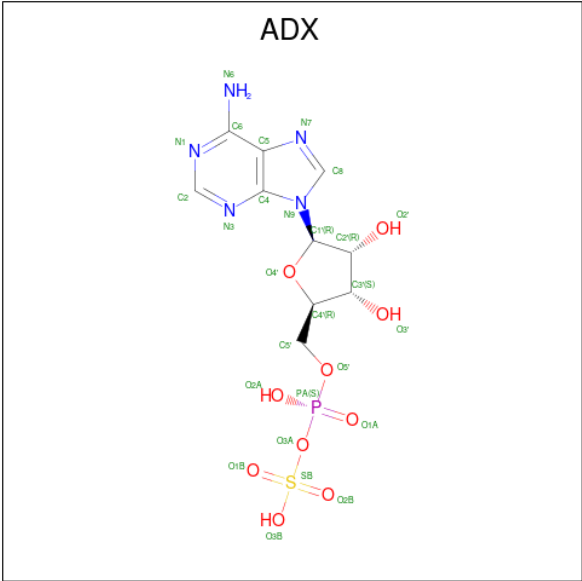
Chain	Residue	Modelled	Actual	Comment	Reference
A	48	MET	-	initiating methionine	UNP Q8SAG1
A	450	LEU	-	expression tag	UNP Q8SAG1
A	451	SER	-	expression tag	UNP Q8SAG1
B	48	MET	-	initiating methionine	UNP Q8SAG1
B	450	LEU	-	expression tag	UNP Q8SAG1
B	451	SER	-	expression tag	UNP Q8SAG1
C	48	MET	-	initiating methionine	UNP Q8SAG1
C	450	LEU	-	expression tag	UNP Q8SAG1
C	451	SER	-	expression tag	UNP Q8SAG1
D	48	MET	-	initiating methionine	UNP Q8SAG1
D	450	LEU	-	expression tag	UNP Q8SAG1
D	451	SER	-	expression tag	UNP Q8SAG1
E	48	MET	-	initiating methionine	UNP Q8SAG1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	450	LEU	-	expression tag	UNP Q8SAG1
E	451	SER	-	expression tag	UNP Q8SAG1
F	48	MET	-	initiating methionine	UNP Q8SAG1
F	450	LEU	-	expression tag	UNP Q8SAG1
F	451	SER	-	expression tag	UNP Q8SAG1
G	48	MET	-	initiating methionine	UNP Q8SAG1
G	450	LEU	-	expression tag	UNP Q8SAG1
G	451	SER	-	expression tag	UNP Q8SAG1
H	48	MET	-	initiating methionine	UNP Q8SAG1
H	450	LEU	-	expression tag	UNP Q8SAG1
H	451	SER	-	expression tag	UNP Q8SAG1

- Molecule 2 is ADENOSINE-5'-PHOSPHOSULFATE (CCD ID: ADX) (formula: C₁₀H₁₄N₅O₁₀PS).



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

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

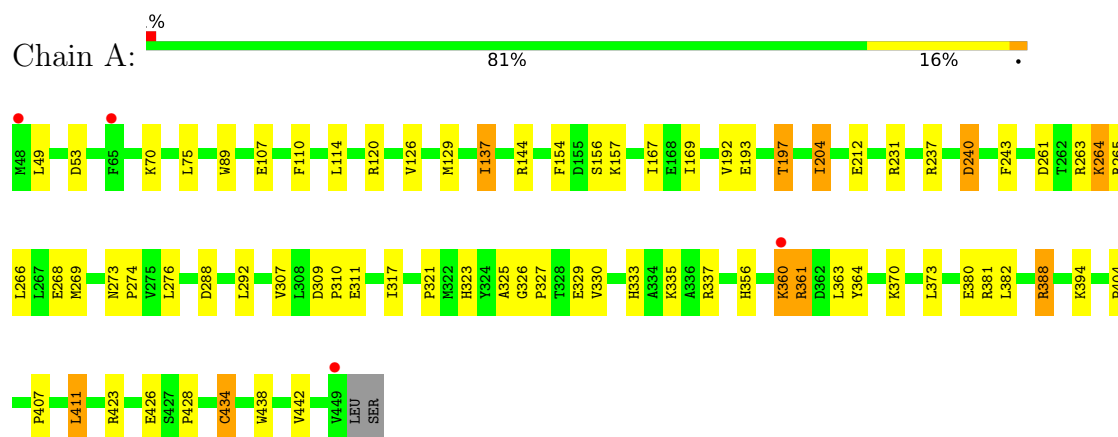
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total	O	0	0
			67	67		
3	B	146	Total	O	0	0
			146	146		
3	C	167	Total	O	0	0
			167	167		
3	D	122	Total	O	0	0
			122	122		
3	E	136	Total	O	0	0
			136	136		
3	F	57	Total	O	0	0
			57	57		
3	G	106	Total	O	0	0
			106	106		
3	H	24	Total	O	0	0
			24	24		

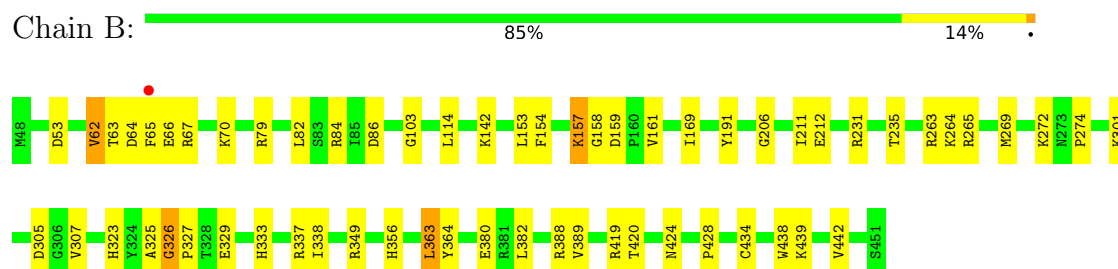
3 Residue-property plots [i](#)

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.

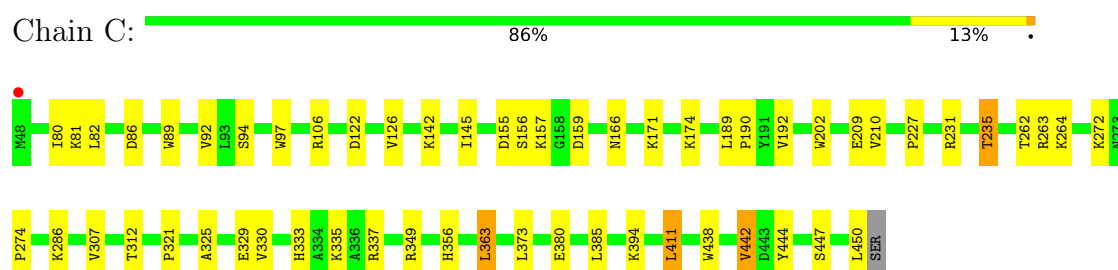
• Molecule 1: ATP sulfurylase



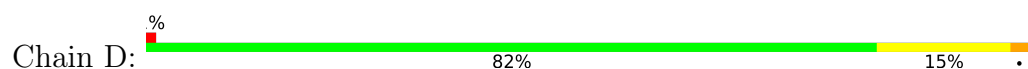
• Molecule 1: ATP sulfurylase

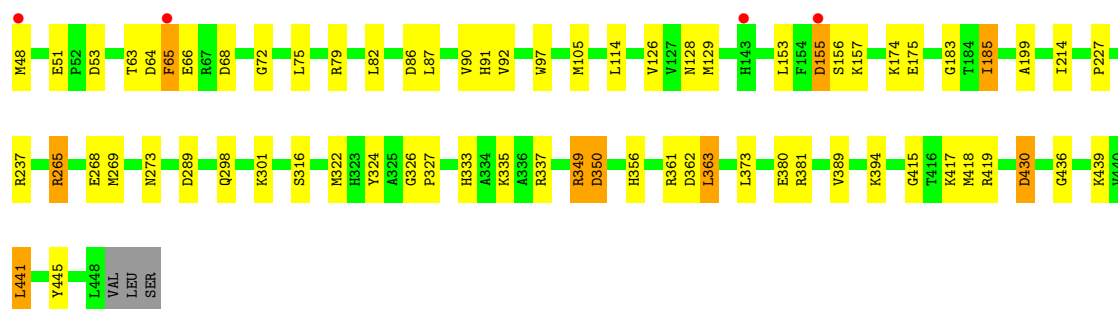


• Molecule 1: ATP sulfurylase

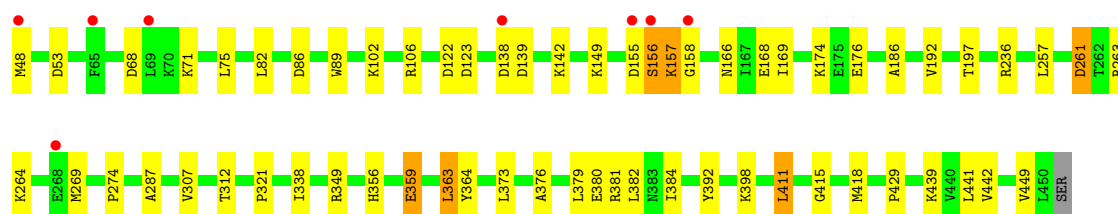
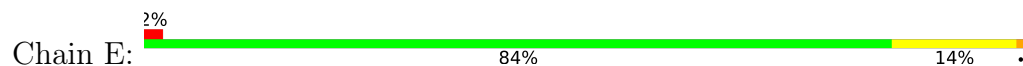


• Molecule 1: ATP sulfurylase

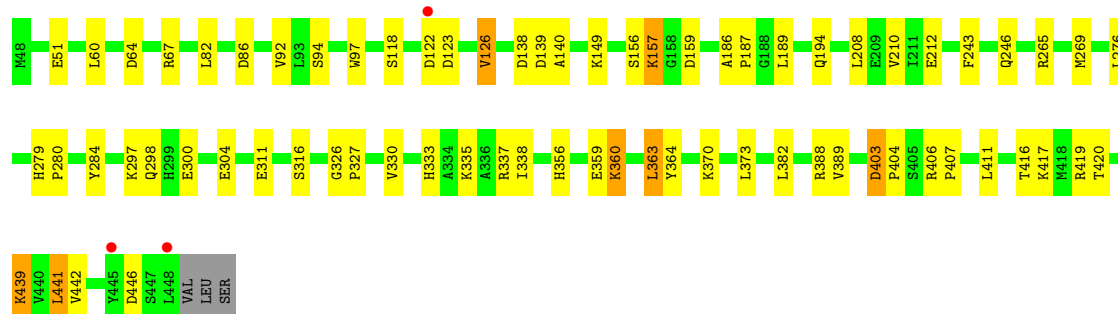
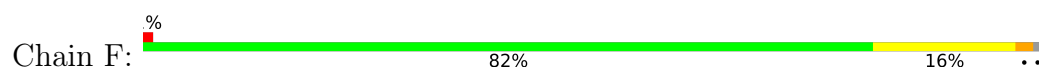




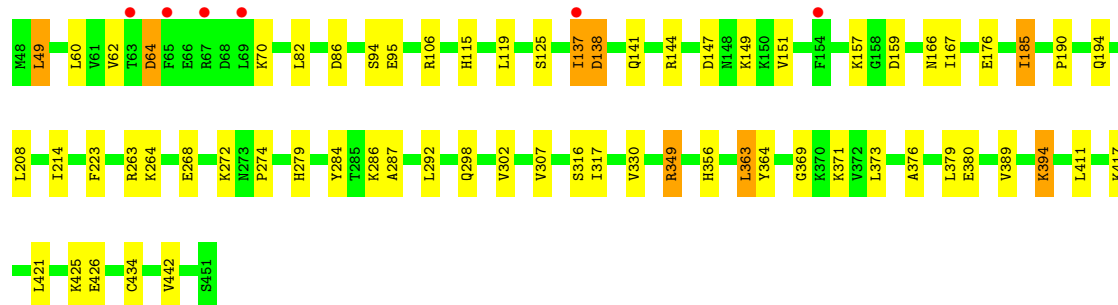
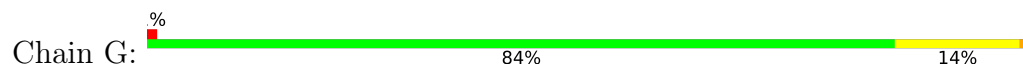
- Molecule 1: ATP sulfurylase



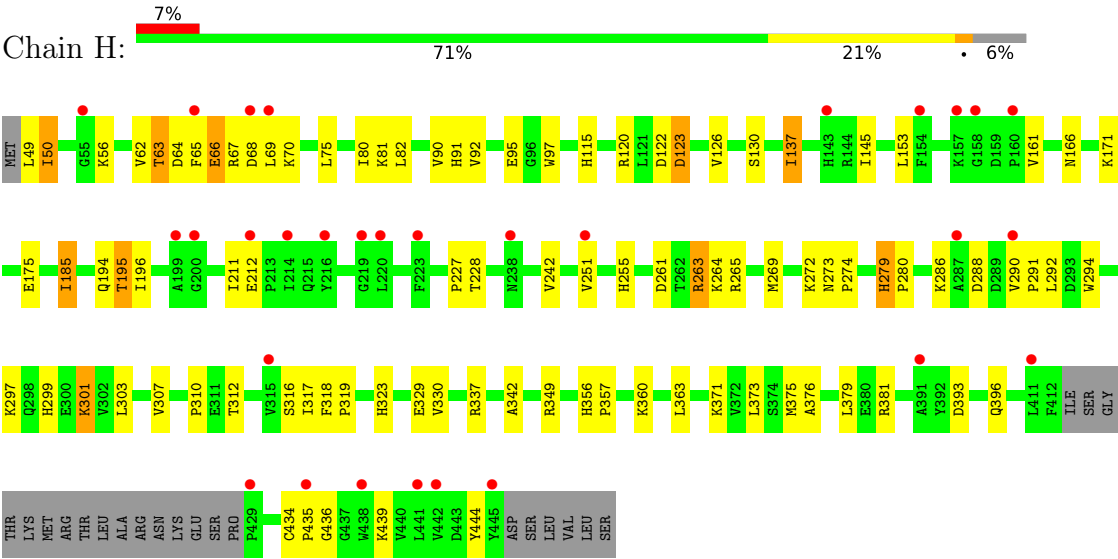
- Molecule 1: ATP sulfurylase



- Molecule 1: ATP sulfurylase



- Molecule 1: ATP sulfurylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	204.27Å 230.75Å 159.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.21 – 2.48 48.21 – 2.48	Depositor EDS
% Data completeness (in resolution range)	93.5 (48.21-2.48) 88.6 (48.21-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.173 , 0.222 0.188 , 0.234	Depositor DCC
R_{free} test set	6239 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26495	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4649e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.48	0/3278	0.85	4/4447 (0.1%)
1	B	0.49	0/3306	0.86	2/4485 (0.0%)
1	C	0.55	0/3286	0.84	1/4458 (0.0%)
1	D	0.52	0/3271	0.86	5/4437 (0.1%)
1	E	0.52	0/3286	0.88	4/4458 (0.1%)
1	F	0.46	0/3271	0.86	5/4437 (0.1%)
1	G	0.51	0/3292	0.86	1/4466 (0.0%)
1	H	0.40	0/3116	0.85	4/4228 (0.1%)
All	All	0.50	0/26106	0.86	26/35416 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	123	ASP	N-CA-C	-9.34	101.89	113.38
1	E	158	GLY	N-CA-C	7.66	125.47	114.67
1	A	361	ARG	N-CA-C	-7.08	98.41	108.96
1	F	189	LEU	CA-C-N	7.06	126.58	119.24
1	F	189	LEU	C-N-CA	7.06	126.58	119.24
1	F	403	ASP	CA-C-N	6.91	126.61	119.56
1	F	403	ASP	C-N-CA	6.91	126.61	119.56
1	E	186	ALA	N-CA-C	6.32	116.86	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	195	THR	N-CA-C	6.14	123.89	110.80
1	H	290	VAL	CA-C-N	5.80	125.81	119.89
1	H	290	VAL	C-N-CA	5.80	125.81	119.89
1	D	155	ASP	N-CA-C	5.79	118.34	108.90
1	A	434	CYS	CA-C-N	5.77	125.90	119.32
1	A	434	CYS	C-N-CA	5.77	125.90	119.32
1	E	156	SER	CA-C-N	5.56	131.71	121.70
1	E	156	SER	C-N-CA	5.56	131.71	121.70
1	H	66	GLU	N-CA-C	-5.50	105.36	113.61
1	D	350	ASP	CA-C-N	-5.41	114.21	119.78
1	D	350	ASP	C-N-CA	-5.41	114.21	119.78
1	A	360	LYS	N-CA-C	5.34	118.42	107.69
1	C	174	LYS	N-CA-C	5.29	116.74	111.07
1	D	185	ILE	N-CA-C	-5.27	100.48	108.17
1	G	125	SER	N-CA-C	5.17	117.52	110.55
1	D	361	ARG	N-CA-C	5.14	116.96	110.33
1	B	326	GLY	CA-C-N	5.08	124.87	119.28
1	B	326	GLY	C-N-CA	5.08	124.87	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	122	ASP	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3197	0	3190	51	0
1	B	3219	0	3215	36	0
1	C	3205	0	3201	34	0
1	D	3190	0	3181	42	0
1	E	3205	0	3201	36	0
1	F	3190	0	3181	34	0
1	G	3211	0	3206	41	0
1	H	3037	0	3018	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
3	A	67	0	0	8	0
3	B	146	0	0	5	0
3	C	167	0	0	4	0
3	D	122	0	0	8	0
3	E	136	0	0	2	0
3	F	57	0	0	2	0
3	G	106	0	0	8	0
3	H	24	0	0	4	0
All	All	26495	0	25489	325	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 6.

All (325) 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:C:356:HIS:O	3:C:1010:HOH:O	1.80	0.98
1:A:423:ARG:NH2	3:A:1028:HOH:O	2.08	0.85
1:E:156:SER:H	1:E:157:LYS:HB3	1.42	0.85
1:H:166:ASN:ND2	3:H:1022:HOH:O	2.13	0.82
1:D:349:ARG:NH1	3:D:1073:HOH:O	2.13	0.81
1:D:289:ASP:OD2	3:D:1079:HOH:O	1.99	0.79
1:B:63:THR:OG1	1:B:66:GLU:OE2	2.03	0.76
1:D:265:ARG:HG2	1:D:269:MET:HE3	1.68	0.76
1:E:415:GLY:HA2	1:E:418:MET:HE3	1.69	0.75
1:B:263:ARG:NH1	3:B:1102:HOH:O	2.20	0.74
1:E:287:ALA:O	3:E:1034:HOH:O	2.06	0.74
1:B:388:ARG:NH1	3:B:1034:HOH:O	2.12	0.73
1:D:380:GLU:OE1	3:D:1044:HOH:O	2.06	0.72
1:C:263:ARG:NH2	1:C:274:PRO:O	2.24	0.70
1:G:95:GLU:OE2	3:G:1087:HOH:O	2.09	0.69
1:G:64:ASP:N	1:G:64:ASP:OD1	2.25	0.69
1:A:237:ARG:O	1:A:273:ASN:ND2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASP:HB3	1:A:381:ARG:HH21	1.58	0.68
1:B:356:HIS:HA	1:B:363:LEU:HD13	1.74	0.68
1:G:49:LEU:N	3:G:1093:HOH:O	2.15	0.68
1:A:265:ARG:HG2	1:A:269:MET:HE2	1.75	0.68
1:H:291:PRO:HG2	1:H:294:TRP:HD1	1.60	0.67
1:H:297:LYS:NZ	3:H:1020:HOH:O	2.18	0.67
1:C:231:ARG:O	1:C:235:THR:HG22	1.93	0.67
1:H:330:VAL:HG13	1:H:373:LEU:HD13	1.77	0.67
1:G:176:GLU:OE1	3:G:1038:HOH:O	2.12	0.67
1:H:81:LYS:O	3:H:1019:HOH:O	2.13	0.67
1:G:349:ARG:HG2	1:G:389:VAL:HG22	1.76	0.67
1:B:67:ARG:NH1	1:B:211:ILE:O	2.29	0.66
1:H:123:ASP:N	1:H:123:ASP:OD1	2.29	0.66
1:E:155:ASP:CG	1:E:156:SER:HB3	2.21	0.66
1:A:237:ARG:NH1	1:A:311:GLU:O	2.28	0.65
1:A:240:ASP:N	1:A:240:ASP:OD1	2.29	0.65
1:H:63:THR:HG22	1:H:66:GLU:HG3	1.78	0.65
1:A:370:LYS:HG3	3:A:1051:HOH:O	1.96	0.64
1:D:349:ARG:HG2	1:D:389:VAL:HG22	1.80	0.64
1:F:82:LEU:HD22	1:F:86:ASP:HB3	1.80	0.64
1:D:63:THR:OG1	1:D:66:GLU:OE1	2.12	0.64
1:H:303:LEU:HG	1:H:310:PRO:HG3	1.79	0.63
1:H:80:ILE:HD11	1:H:145:ILE:HD11	1.81	0.62
1:D:155:ASP:O	1:D:157:LYS:N	2.32	0.62
1:G:263:ARG:NH2	1:G:274:PRO:O	2.29	0.62
1:E:156:SER:H	1:E:157:LYS:CB	2.14	0.61
1:A:193:GLU:HA	1:A:197:THR:HG23	1.83	0.61
1:D:72:GLY:HA3	1:H:68:ASP:O	2.01	0.61
1:F:265:ARG:HG2	1:F:269:MET:HE3	1.82	0.60
1:A:360:LYS:HE2	3:A:1065:HOH:O	2.02	0.60
1:F:356:HIS:HA	1:F:363:LEU:HD13	1.84	0.60
1:F:416:THR:HG22	1:F:419:ARG:HH21	1.67	0.60
1:E:263:ARG:NH2	1:E:274:PRO:O	2.34	0.60
1:F:370:LYS:HG3	3:F:1006:HOH:O	2.01	0.60
1:E:359:GLU:O	3:E:1113:HOH:O	2.17	0.59
1:D:265:ARG:HH11	1:D:265:ARG:HB2	1.66	0.59
1:G:106:ARG:NH2	1:G:166:ASN:O	2.35	0.59
1:D:237:ARG:O	1:D:273:ASN:ND2	2.36	0.59
1:D:419:ARG:HG3	1:D:445:TYR:CE1	2.38	0.59
1:D:362:ASP:OD2	3:D:1071:HOH:O	2.17	0.58
1:E:149:LYS:HG2	1:E:166:ASN:HA	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HG23	1:A:204:ILE:HD11	1.86	0.58
1:A:356:HIS:HA	1:A:363:LEU:HD13	1.85	0.58
1:D:316:SER:OG	3:D:1012:HOH:O	2.15	0.57
1:A:266:LEU:HA	1:A:269:MET:HE3	1.87	0.57
1:C:80:ILE:HD11	1:C:145:ILE:HD11	1.87	0.57
1:G:263:ARG:NH1	3:G:1081:HOH:O	2.31	0.56
1:C:155:ASP:HB3	1:C:157:LYS:H	1.70	0.56
1:D:356:HIS:HA	1:D:363:LEU:HD13	1.87	0.56
1:D:53:ASP:HB3	1:D:381:ARG:HH21	1.69	0.56
1:E:89:TRP:CE2	1:E:321:PRO:HG2	2.41	0.56
1:F:67:ARG:HH21	1:F:212:GLU:HA	1.70	0.56
1:H:294:TRP:CE3	1:H:444:TYR:HB2	2.40	0.56
1:D:128:ASN:OD1	3:D:1106:HOH:O	2.18	0.56
1:H:62:VAL:HG11	1:H:70:LYS:HG3	1.87	0.56
1:H:242:VAL:HB	1:H:342:ALA:HA	1.89	0.55
1:A:307:VAL:HG21	1:A:434:CYS:HB3	1.87	0.55
1:D:415:GLY:HA2	1:D:418:MET:HE3	1.88	0.55
1:B:265:ARG:HG2	1:B:269:MET:HE3	1.88	0.55
1:C:356:HIS:HA	1:C:363:LEU:HD13	1.88	0.55
1:G:82:LEU:HD22	1:G:86:ASP:HB3	1.87	0.55
1:D:350:ASP:OD2	3:D:1005:HOH:O	2.17	0.54
3:F:1034:HOH:O	1:G:115:HIS:HD2	1.91	0.54
1:H:65:PHE:CZ	1:H:67:ARG:HB3	2.43	0.54
1:E:356:HIS:HA	1:E:363:LEU:HD13	1.90	0.54
1:B:82:LEU:HD22	1:B:86:ASP:HB3	1.90	0.53
1:D:105:MET:HE3	1:D:129:MET:HE2	1.89	0.53
1:F:360:LYS:HZ2	1:F:360:LYS:HA	1.71	0.53
1:H:67:ARG:HG3	1:H:211:ILE:HG23	1.89	0.53
1:B:301:LYS:HE2	1:B:439:LYS:HZ1	1.72	0.53
1:E:156:SER:N	1:E:157:LYS:HB3	2.19	0.53
1:A:380:GLU:OE1	3:A:1053:HOH:O	2.19	0.53
1:E:53:ASP:HB3	1:E:381:ARG:HH21	1.73	0.53
1:B:325:ALA:HB3	1:B:329:GLU:HB2	1.91	0.52
1:G:380:GLU:H	1:G:380:GLU:CD	2.17	0.52
1:E:106:ARG:NH2	1:E:166:ASN:O	2.42	0.52
1:G:287:ALA:HA	3:G:1069:HOH:O	2.09	0.52
1:A:144:ARG:NH2	3:A:1044:HOH:O	2.41	0.52
1:A:129:MET:HE3	1:A:129:MET:HA	1.92	0.52
1:B:79:ARG:HD2	1:B:154:PHE:CE2	2.44	0.52
1:C:209:GLU:OE2	3:C:1152:HOH:O	2.19	0.52
1:A:156:SER:HB2	1:A:157:LYS:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LEU:HD22	1:D:86:ASP:HB3	1.92	0.52
1:F:194:GLN:HG3	1:F:284:TYR:CE1	2.44	0.52
1:A:333:HIS:O	1:A:337:ARG:HD3	2.10	0.52
1:G:356:HIS:HA	1:G:363:LEU:HD13	1.91	0.52
1:G:371:LYS:NZ	3:G:1048:HOH:O	2.43	0.52
1:C:190:PRO:HG3	1:C:286:LYS:HD3	1.92	0.51
1:D:436:GLY:HA2	1:D:439:LYS:HD2	1.93	0.51
1:A:193:GLU:HA	1:A:197:THR:CG2	2.40	0.51
1:E:263:ARG:HG2	1:E:264:LYS:HE2	1.91	0.51
1:C:330:VAL:HG13	1:C:373:LEU:HD13	1.92	0.51
1:G:137:ILE:HG23	1:G:141:GLN:HB2	1.91	0.51
1:D:91:HIS:HA	1:D:214:ILE:HD13	1.92	0.51
1:C:155:ASP:HB2	1:C:159:ASP:H	1.76	0.51
1:G:292:LEU:HD21	1:G:317:ILE:HD13	1.91	0.51
1:H:280:PRO:HD2	1:H:316:SER:O	2.11	0.51
1:C:171:LYS:NZ	3:C:1049:HOH:O	2.34	0.50
1:C:380:GLU:CD	1:C:380:GLU:H	2.20	0.50
1:C:380:GLU:OE1	3:C:1070:HOH:O	2.18	0.50
1:D:65:PHE:CD2	1:D:65:PHE:N	2.79	0.50
1:B:265:ARG:NH1	3:B:1049:HOH:O	1.92	0.50
1:B:157:LYS:O	1:B:159:ASP:N	2.44	0.50
1:A:89:TRP:CE2	1:A:321:PRO:HG2	2.46	0.50
1:E:82:LEU:HD22	1:E:86:ASP:HB3	1.94	0.50
1:B:439:LYS:HA	1:B:442:VAL:HG22	1.94	0.49
1:F:330:VAL:HG13	1:F:373:LEU:HD13	1.94	0.49
1:H:292:LEU:HD21	1:H:317:ILE:HD13	1.93	0.49
1:C:122:ASP:O	1:D:301:LYS:NZ	2.34	0.49
1:E:380:GLU:H	1:E:380:GLU:CD	2.21	0.49
1:G:60:LEU:HD13	1:G:208:LEU:HB3	1.95	0.49
1:H:376:ALA:HB3	1:H:379:LEU:HD12	1.93	0.49
1:C:333:HIS:O	1:C:337:ARG:HD3	2.12	0.49
1:G:279:HIS:HD2	1:G:316:SER:O	1.95	0.49
1:D:430:ASP:OD2	1:D:430:ASP:N	2.45	0.49
1:E:89:TRP:CZ2	1:E:321:PRO:HG2	2.47	0.49
1:H:82:LEU:HD21	1:H:90:VAL:HG21	1.94	0.49
1:H:194:GLN:O	1:H:196:ILE:N	2.43	0.49
1:H:294:TRP:CE3	1:H:297:LYS:HE3	2.48	0.48
1:A:382:LEU:O	3:A:1004:HOH:O	2.20	0.48
1:B:191:TYR:OH	3:B:1052:HOH:O	2.16	0.48
1:E:192:VAL:HG12	1:E:197:THR:HG23	1.96	0.48
1:C:89:TRP:CZ2	1:C:321:PRO:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:330:VAL:HG13	1:G:373:LEU:HD13	1.95	0.48
3:A:1050:HOH:O	1:H:115:HIS:HD2	1.95	0.48
1:F:360:LYS:HA	1:F:360:LYS:NZ	2.28	0.48
1:G:151:VAL:HG13	1:G:167:ILE:HD13	1.96	0.48
1:G:141:GLN:HG2	1:G:144:ARG:HH21	1.78	0.48
1:A:325:ALA:HB3	1:A:329:GLU:HB2	1.95	0.48
1:A:394:LYS:HD2	1:A:411:LEU:HD13	1.96	0.48
1:A:361:ARG:NH2	1:H:175:GLU:OE1	2.47	0.48
1:A:363:LEU:HB3	1:A:364:TYR:CD2	2.48	0.48
1:C:325:ALA:HB3	1:C:329:GLU:HB2	1.96	0.48
1:A:192:VAL:HG12	1:A:197:THR:HG22	1.96	0.47
1:F:279:HIS:HD2	1:F:316:SER:O	1.97	0.47
1:C:189:LEU:HB2	1:C:192:VAL:HB	1.96	0.47
1:H:65:PHE:CE2	1:H:67:ARG:HB3	2.49	0.47
1:C:106:ARG:NH2	1:C:166:ASN:O	2.47	0.47
1:D:183:GLY:O	1:E:176:GLU:HA	2.14	0.47
1:G:417:LYS:O	1:G:421:LEU:HG	2.15	0.47
1:C:92:VAL:HG13	1:C:97:TRP:HB2	1.96	0.47
1:D:97:TRP:CE2	1:D:227:PRO:HD3	2.49	0.47
1:H:64:ASP:HA	1:H:65:PHE:HA	1.58	0.47
1:H:263:ARG:NH2	1:H:274:PRO:O	2.42	0.47
1:H:318:PHE:HA	1:H:319:PRO:HD3	1.78	0.47
1:G:307:VAL:HG21	1:G:434:CYS:HB3	1.97	0.47
1:D:333:HIS:O	1:D:337:ARG:HD3	2.15	0.46
1:G:166:ASN:ND2	3:G:1078:HOH:O	2.48	0.46
1:B:428:PRO:HD3	1:B:438:TRP:CZ2	2.50	0.46
1:E:373:LEU:HG	1:E:384:ILE:HD12	1.97	0.46
1:F:280:PRO:HD2	1:F:316:SER:O	2.15	0.46
1:D:439:LYS:HG3	3:D:1060:HOH:O	2.15	0.46
1:B:301:LYS:CE	1:B:439:LYS:HZ1	2.29	0.46
1:B:380:GLU:H	1:B:380:GLU:CD	2.24	0.46
1:C:82:LEU:HD22	1:C:86:ASP:HB3	1.97	0.46
1:D:68:ASP:HB2	1:H:69:LEU:HD12	1.97	0.46
1:A:380:GLU:HG2	1:H:120:ARG:NH2	2.30	0.46
1:B:82:LEU:HD11	1:B:153:LEU:HB3	1.98	0.46
1:F:326:GLY:HA3	1:F:327:PRO:HD3	1.81	0.46
1:G:376:ALA:HB3	1:G:379:LEU:HD12	1.97	0.46
1:D:326:GLY:HA3	1:D:327:PRO:HD3	1.80	0.46
1:E:82:LEU:HB3	1:E:86:ASP:HB2	1.98	0.46
1:A:330:VAL:HG13	1:A:373:LEU:HD13	1.97	0.46
1:B:62:VAL:HG11	1:B:70:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:243:PHE:CZ	1:F:276:LEU:HB2	2.51	0.46
1:B:263:ARG:HG2	1:B:264:LYS:HE2	1.97	0.45
1:D:298:GLN:HG3	1:D:441:LEU:HD13	1.98	0.45
1:H:82:LEU:HD11	1:H:153:LEU:HB3	1.98	0.45
1:B:333:HIS:O	1:B:337:ARG:HD3	2.16	0.45
1:C:89:TRP:CE2	1:C:321:PRO:HG2	2.51	0.45
1:G:144:ARG:NH1	3:G:1058:HOH:O	2.42	0.45
1:D:174:LYS:NZ	1:D:199:ALA:O	2.45	0.45
1:H:92:VAL:HG13	1:H:97:TRP:HB2	1.97	0.45
1:A:326:GLY:HA3	1:A:327:PRO:HD3	1.83	0.45
1:F:92:VAL:HG13	1:F:97:TRP:HB2	1.99	0.45
1:F:439:LYS:O	1:F:442:VAL:HG22	2.17	0.45
1:G:425:LYS:HB3	1:G:425:LYS:HE2	1.56	0.45
1:E:106:ARG:HB3	1:E:168:GLU:CD	2.42	0.45
1:G:194:GLN:HG3	1:G:284:TYR:CE1	2.52	0.45
1:A:137:ILE:CG2	1:A:204:ILE:HD11	2.47	0.45
1:F:417:LYS:HA	1:F:420:THR:HG22	1.99	0.45
1:G:298:GLN:O	1:G:302:VAL:HG23	2.17	0.45
1:H:185:ILE:HD13	1:H:185:ILE:HA	1.85	0.44
1:B:264:LYS:HA	1:B:264:LYS:HD3	1.58	0.44
1:E:263:ARG:NH2	1:E:312:THR:HB	2.33	0.44
1:F:333:HIS:O	1:F:337:ARG:HD3	2.17	0.44
1:H:286:LYS:HD2	1:H:288:ASP:HB3	1.99	0.44
1:A:156:SER:HA	1:A:157:LYS:HA	1.61	0.44
1:A:380:GLU:CD	1:A:380:GLU:H	2.26	0.44
1:C:444:TYR:O	1:C:447:SER:HB2	2.18	0.44
1:G:185:ILE:HA	1:G:185:ILE:HD13	1.75	0.44
1:A:263:ARG:NH2	1:A:274:PRO:O	2.40	0.44
1:B:142:LYS:HG3	1:B:169:ILE:HD13	1.98	0.44
1:H:435:PRO:O	1:H:439:LYS:HG3	2.18	0.44
1:F:157:LYS:O	1:F:159:ASP:N	2.50	0.44
1:C:394:LYS:HD2	1:C:411:LEU:HD22	2.00	0.44
1:C:438:TRP:O	1:C:442:VAL:HG13	2.17	0.44
1:D:86:ASP:O	1:D:90:VAL:HG23	2.17	0.44
1:E:122:ASP:OD2	1:E:122:ASP:N	2.51	0.44
1:H:279:HIS:HB3	1:H:337:ARG:HH21	1.83	0.44
1:B:79:ARG:HD2	1:B:154:PHE:CZ	2.52	0.44
1:H:49:LEU:HD12	1:H:50:ILE:H	1.83	0.44
1:H:130:SER:N	3:H:1005:HOH:O	2.37	0.44
1:H:323:HIS:HB2	1:H:329:GLU:CD	2.43	0.43
1:A:107:GLU:OE1	1:H:371:LYS:NZ	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:LEU:HD11	1:H:75:LEU:HD11	1.99	0.43
1:E:142:LYS:HD2	1:E:169:ILE:HG21	1.98	0.43
1:A:323:HIS:HB2	1:A:329:GLU:CD	2.43	0.43
1:G:369:GLY:O	1:G:373:LEU:HB2	2.18	0.43
1:H:263:ARG:NH2	1:H:312:THR:HB	2.33	0.43
1:H:434:CYS:HA	1:H:435:PRO:HD3	1.89	0.43
1:B:231:ARG:O	1:B:235:THR:HG22	2.19	0.43
1:F:338:ILE:HG12	1:F:382:LEU:HD13	2.00	0.43
1:G:62:VAL:HG11	1:G:70:LYS:HG3	2.00	0.43
1:A:309:ASP:HA	1:A:310:PRO:HD2	1.90	0.43
1:B:326:GLY:HA3	1:B:327:PRO:HD3	1.79	0.43
1:B:157:LYS:C	1:B:159:ASP:H	2.25	0.43
1:B:338:ILE:HG12	1:B:382:LEU:HD13	2.01	0.43
1:C:263:ARG:NH2	1:C:312:THR:HB	2.34	0.43
1:E:156:SER:H	1:E:157:LYS:CA	2.31	0.43
1:A:110:PHE:CZ	1:A:114:LEU:HD11	2.53	0.43
1:A:169:ILE:HG13	1:A:204:ILE:HG23	1.99	0.43
1:E:392:TYR:CZ	1:E:429:PRO:HB2	2.54	0.43
1:A:404:PRO:O	1:A:407:PRO:HD3	2.19	0.42
1:C:142:LYS:HE2	1:C:202:TRP:CZ2	2.54	0.42
1:C:394:LYS:HD2	1:C:411:LEU:HD13	2.00	0.42
1:D:105:MET:CE	1:D:129:MET:HE2	2.49	0.42
1:H:95:GLU:HB3	1:H:227:PRO:HD2	2.00	0.42
1:H:263:ARG:HH21	1:H:274:PRO:C	2.27	0.42
1:H:307:VAL:HG21	1:H:434:CYS:HB3	2.01	0.42
1:A:264:LYS:O	1:A:268:GLU:HG3	2.19	0.42
1:F:67:ARG:HE	1:F:212:GLU:HG2	1.83	0.42
1:H:137:ILE:HD13	1:H:137:ILE:HA	1.84	0.42
1:B:263:ARG:NH2	1:B:274:PRO:O	2.33	0.42
1:C:411:LEU:HD12	1:C:411:LEU:HA	1.80	0.42
1:E:264:LYS:HD3	1:E:264:LYS:HA	1.74	0.42
1:G:119:LEU:HD23	1:G:119:LEU:HA	1.86	0.42
1:A:49:LEU:HD22	1:A:231:ARG:HG2	2.01	0.42
1:F:64:ASP:HA	1:F:67:ARG:NH1	2.34	0.42
1:E:71:LYS:O	1:E:75:LEU:HG	2.20	0.42
1:F:403:ASP:OD1	1:F:406:ARG:HD3	2.19	0.42
1:B:307:VAL:HG21	1:B:434:CYS:HB3	2.00	0.42
1:B:363:LEU:HB3	1:B:364:TYR:CD2	2.55	0.42
1:E:155:ASP:HA	1:E:156:SER:HA	1.64	0.42
1:G:137:ILE:HD13	1:G:137:ILE:HA	1.79	0.42
1:G:363:LEU:HB3	1:G:364:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:265:ARG:O	1:H:269:MET:HB2	2.19	0.42
1:A:373:LEU:HD12	1:A:373:LEU:HA	1.93	0.42
1:A:381:ARG:HD3	3:A:1053:HOH:O	2.19	0.42
1:F:298:GLN:HG3	1:F:441:LEU:HD13	2.02	0.42
1:A:70:LYS:HD3	1:A:70:LYS:HA	1.84	0.42
1:C:94:SER:HB3	1:C:210:VAL:HG21	2.01	0.42
1:D:175:GLU:HG3	1:D:185:ILE:HD12	2.02	0.42
1:E:376:ALA:HB3	1:E:379:LEU:HD12	2.01	0.42
1:F:186:ALA:HA	1:F:187:PRO:HD3	1.93	0.42
1:C:264:LYS:HE3	1:C:264:LYS:HB2	1.85	0.42
1:F:118:SER:HB2	1:F:126:VAL:HG13	2.02	0.42
1:H:356:HIS:HA	1:H:357:PRO:HD3	1.95	0.42
1:A:265:ARG:HE	1:A:265:ARG:HB2	1.52	0.41
1:A:428:PRO:HD3	1:A:438:TRP:CZ2	2.55	0.41
1:C:81:LYS:HE3	1:C:156:SER:HA	2.01	0.41
1:F:94:SER:HB3	1:F:210:VAL:HG21	2.01	0.41
1:F:194:GLN:HG3	1:F:284:TYR:CZ	2.55	0.41
1:H:301:LYS:HG2	1:H:436:GLY:C	2.45	0.41
1:H:153:LEU:O	1:H:161:VAL:HG22	2.20	0.41
1:F:411:LEU:HA	1:F:411:LEU:HD12	1.88	0.41
1:G:190:PRO:HG3	1:G:286:LYS:HD3	2.03	0.41
1:G:394:LYS:CD	1:G:411:LEU:HG	2.50	0.41
1:H:251:VAL:HG13	1:H:255:HIS:HB2	2.02	0.41
1:H:436:GLY:HA2	1:H:439:LYS:HD2	2.02	0.41
1:A:292:LEU:HD21	1:A:317:ILE:HD13	2.03	0.41
1:E:411:LEU:HA	1:E:411:LEU:HD12	1.72	0.41
1:G:70:LYS:HA	1:G:70:LYS:HD3	1.85	0.41
1:D:92:VAL:HG13	1:D:97:TRP:HB2	2.03	0.41
1:D:373:LEU:HD12	1:D:373:LEU:HA	1.90	0.41
1:E:338:ILE:HD11	1:E:382:LEU:HB2	2.03	0.41
1:H:280:PRO:HG3	1:H:299:HIS:CD2	2.55	0.41
1:A:75:LEU:HD23	1:A:154:PHE:HZ	1.86	0.41
1:A:388:ARG:H	1:A:388:ARG:HG2	1.69	0.41
1:C:97:TRP:CE2	1:C:227:PRO:HD3	2.55	0.41
1:F:363:LEU:HB3	1:F:364:TYR:CD2	2.55	0.41
1:G:223:PHE:O	1:G:316:SER:HB2	2.20	0.41
1:B:323:HIS:HB2	1:B:329:GLU:CD	2.45	0.41
1:F:138:ASP:HB3	1:F:140:ALA:H	1.86	0.41
1:H:286:LYS:HG3	1:H:288:ASP:HB3	2.03	0.41
1:A:120:ARG:NH2	1:H:375:MET:O	2.52	0.41
1:B:103:GLY:HA3	1:B:206:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:GLU:OE1	3:B:1088:HOH:O	2.21	0.41
1:B:420:THR:O	1:B:424:ASN:ND2	2.50	0.41
1:F:419:ARG:HG3	1:F:419:ARG:HH11	1.86	0.41
1:G:60:LEU:HB2	1:G:94:SER:HA	2.01	0.41
1:G:138:ASP:HB2	1:G:141:GLN:OE1	2.20	0.41
1:H:291:PRO:HG2	1:H:294:TRP:CD1	2.48	0.41
1:C:262:THR:HG23	1:C:385:LEU:HD13	2.03	0.41
1:D:394:LYS:HE3	1:D:394:LYS:HB2	1.71	0.41
1:H:56:LYS:HD3	1:H:56:LYS:HA	1.89	0.41
1:B:363:LEU:HB3	1:B:364:TYR:CE2	2.56	0.40
1:F:404:PRO:O	1:F:407:PRO:HD3	2.20	0.40
1:H:280:PRO:HG3	1:H:299:HIS:HD2	1.86	0.40
1:D:322:MET:HG2	1:D:324:TYR:CZ	2.56	0.40
1:A:243:PHE:CZ	1:A:276:LEU:HB2	2.57	0.40
1:E:363:LEU:HB3	1:E:364:TYR:CD2	2.56	0.40
1:E:123:ASP:OD1	1:E:123:ASP:N	2.51	0.40
1:E:257:LEU:O	1:E:261:ASP:HB2	2.21	0.40
1:D:82:LEU:HD21	1:D:153:LEU:HD13	2.03	0.40
1:F:60:LEU:HD13	1:F:208:LEU:HB3	2.03	0.40
1:H:91:HIS:NE2	1:H:95:GLU:OE2	2.53	0.40
1:H:393:ASP:OD2	1:H:396:GLN:NE2	2.52	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	400/404 (99%)	394 (98%)	6 (2%)	0	100	100
1	B	404/404 (100%)	397 (98%)	5 (1%)	2 (0%)	24	40
1	C	401/404 (99%)	396 (99%)	5 (1%)	0	100	100
1	D	399/404 (99%)	388 (97%)	10 (2%)	1 (0%)	36	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	401/404 (99%)	396 (99%)	5 (1%)	0	100	100
1	F	399/404 (99%)	390 (98%)	9 (2%)	0	100	100
1	G	402/404 (100%)	392 (98%)	10 (2%)	0	100	100
1	H	377/404 (93%)	360 (96%)	16 (4%)	1 (0%)	36	53
All	All	3183/3232 (98%)	3113 (98%)	66 (2%)	4 (0%)	48	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	156	SER
1	H	195	THR
1	B	157	LYS
1	B	158	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	344/346 (99%)	329 (96%)	15 (4%)	25	47
1	B	348/346 (101%)	333 (96%)	15 (4%)	26	48
1	C	345/346 (100%)	335 (97%)	10 (3%)	37	62
1	D	343/346 (99%)	327 (95%)	16 (5%)	23	44
1	E	345/346 (100%)	325 (94%)	20 (6%)	18	35
1	F	343/346 (99%)	323 (94%)	20 (6%)	18	35
1	G	346/346 (100%)	328 (95%)	18 (5%)	21	39
1	H	325/346 (94%)	304 (94%)	21 (6%)	15	30
All	All	2739/2768 (99%)	2604 (95%)	135 (5%)	22	42

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	VAL
1	A	137	ILE
1	A	167	ILE
1	A	197	THR
1	A	204	ILE
1	A	212	GLU
1	A	240	ASP
1	A	261	ASP
1	A	264	LYS
1	A	288	ASP
1	A	335	LYS
1	A	388	ARG
1	A	411	LEU
1	A	426	GLU
1	A	442	VAL
1	B	53[A]	ASP
1	B	53[B]	ASP
1	B	62	VAL
1	B	64	ASP
1	B	65	PHE
1	B	84	ARG
1	B	114	LEU
1	B	161	VAL
1	B	212	GLU
1	B	272	LYS
1	B	305	ASP
1	B	349	ARG
1	B	363	LEU
1	B	389	VAL
1	B	419	ARG
1	C	126	VAL
1	C	235	THR
1	C	272	LYS
1	C	307	VAL
1	C	335	LYS
1	C	349	ARG
1	C	363	LEU
1	C	411	LEU
1	C	442	VAL
1	C	450	LEU
1	D	48	MET
1	D	51	GLU
1	D	64	ASP

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Mol	Chain	Res	Type
1	D	65	PHE
1	D	79	ARG
1	D	87	LEU
1	D	114	LEU
1	D	126	VAL
1	D	265	ARG
1	D	268	GLU
1	D	335	LYS
1	D	349	ARG
1	D	363	LEU
1	D	417	LYS
1	D	430	ASP
1	D	441	LEU
1	E	48	MET
1	E	68	ASP
1	E	102	LYS
1	E	138	ASP
1	E	139	ASP
1	E	157	LYS
1	E	174	LYS
1	E	236	ARG
1	E	261	ASP
1	E	269	MET
1	E	307	VAL
1	E	349	ARG
1	E	359	GLU
1	E	363	LEU
1	E	398	LYS
1	E	411	LEU
1	E	439	LYS
1	E	441	LEU
1	E	442	VAL
1	E	449	VAL
1	F	51	GLU
1	F	126	VAL
1	F	139	ASP
1	F	149	LYS
1	F	156	SER
1	F	157	LYS
1	F	246	GLN
1	F	297	LYS
1	F	300	GLU

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Mol	Chain	Res	Type
1	F	304	GLU
1	F	311	GLU
1	F	335	LYS
1	F	359	GLU
1	F	360	LYS
1	F	363	LEU
1	F	388	ARG
1	F	389	VAL
1	F	439	LYS
1	F	441	LEU
1	F	446	ASP
1	G	49	LEU
1	G	64	ASP
1	G	137	ILE
1	G	138	ASP
1	G	147	ASP
1	G	149	LYS
1	G	157	LYS
1	G	159	ASP
1	G	185	ILE
1	G	214	ILE
1	G	264	LYS
1	G	268	GLU
1	G	272	LYS
1	G	349	ARG
1	G	363	LEU
1	G	394	LYS
1	G	426	GLU
1	G	442	VAL
1	H	50	ILE
1	H	63	THR
1	H	122	ASP
1	H	123	ASP
1	H	126	VAL
1	H	137	ILE
1	H	171	LYS
1	H	185	ILE
1	H	212	GLU
1	H	228	THR
1	H	261	ASP
1	H	263	ARG
1	H	264	LYS

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Mol	Chain	Res	Type
1	H	272	LYS
1	H	273	ASN
1	H	279	HIS
1	H	301	LYS
1	H	349	ARG
1	H	360	LYS
1	H	363	LEU
1	H	381	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	128	ASN
1	A	331	GLN
1	A	383	ASN
1	B	238	ASN
1	B	383	ASN
1	C	201	ASN
1	C	383	ASN
1	D	323	HIS
1	D	383	ASN
1	E	383	ASN
1	E	396	GLN
1	G	148	ASN
1	H	115	HIS
1	H	117	ASN
1	H	128	ASN
1	H	299	HIS
1	H	323	HIS
1	H	331	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	ADX	B	900	-	29,29,29	1.63	6 (20%)	42,45,45	2.07	11 (26%)
2	ADX	A	900	-	29,29,29	1.66	6 (20%)	42,45,45	1.97	9 (21%)
2	ADX	C	900	-	29,29,29	1.57	4 (13%)	42,45,45	2.09	9 (21%)
2	ADX	G	900	-	29,29,29	1.70	6 (20%)	42,45,45	2.03	9 (21%)
2	ADX	F	900	-	29,29,29	1.74	6 (20%)	42,45,45	1.92	9 (21%)
2	ADX	E	900	-	29,29,29	1.66	6 (20%)	42,45,45	1.88	11 (26%)
2	ADX	H	900	-	29,29,29	1.77	6 (20%)	42,45,45	2.00	9 (21%)
2	ADX	D	900	-	29,29,29	1.64	7 (24%)	42,45,45	1.86	11 (26%)

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	ADX	B	900	-	-	1/10/32/32	0/3/3/3
2	ADX	A	900	-	-	0/10/32/32	0/3/3/3
2	ADX	C	900	-	-	3/10/32/32	0/3/3/3
2	ADX	G	900	-	-	0/10/32/32	0/3/3/3
2	ADX	F	900	-	-	3/10/32/32	0/3/3/3
2	ADX	E	900	-	-	1/10/32/32	0/3/3/3
2	ADX	H	900	-	-	3/10/32/32	0/3/3/3
2	ADX	D	900	-	-	1/10/32/32	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	ADX	C6-N6	4.18	1.44	1.34
2	H	900	ADX	C6-N6	4.10	1.44	1.34
2	F	900	ADX	C6-N6	4.00	1.44	1.34
2	H	900	ADX	O3A-SB	-3.88	1.48	1.65
2	B	900	ADX	O3A-SB	-3.86	1.48	1.65
2	G	900	ADX	C6-N6	3.83	1.44	1.34
2	D	900	ADX	C6-N6	3.82	1.44	1.34
2	G	900	ADX	O3A-SB	-3.80	1.49	1.65
2	A	900	ADX	C6-N6	3.78	1.43	1.34
2	C	900	ADX	C6-N6	3.73	1.43	1.34
2	B	900	ADX	C6-N6	3.64	1.43	1.34
2	E	900	ADX	O3A-SB	-3.61	1.49	1.65
2	F	900	ADX	O3A-SB	-3.56	1.50	1.65
2	A	900	ADX	O3A-SB	-3.50	1.50	1.65
2	C	900	ADX	O3A-SB	-3.46	1.50	1.65
2	D	900	ADX	O3A-SB	-3.44	1.50	1.65
2	H	900	ADX	O2'-C2'	-3.28	1.34	1.43
2	F	900	ADX	O2'-C2'	-3.25	1.34	1.43
2	D	900	ADX	O2'-C2'	-3.06	1.35	1.43
2	A	900	ADX	O2'-C2'	-3.04	1.35	1.43
2	C	900	ADX	O2'-C2'	-3.02	1.35	1.43
2	H	900	ADX	C5'-C4'	-3.00	1.42	1.51
2	G	900	ADX	O2'-C2'	-2.96	1.35	1.43
2	F	900	ADX	C5'-C4'	-2.92	1.42	1.51
2	E	900	ADX	O2'-C2'	-2.90	1.35	1.43
2	A	900	ADX	C5'-C4'	-2.83	1.43	1.51
2	B	900	ADX	C5'-C4'	-2.75	1.43	1.51
2	B	900	ADX	O2'-C2'	-2.65	1.36	1.43
2	G	900	ADX	C5'-C4'	-2.64	1.43	1.51
2	E	900	ADX	C5'-C4'	-2.59	1.43	1.51
2	C	900	ADX	C5'-C4'	-2.51	1.44	1.51
2	D	900	ADX	C5'-C4'	-2.44	1.44	1.51
2	G	900	ADX	C1'-N9	-2.38	1.39	1.46
2	H	900	ADX	C2'-C3'	-2.34	1.47	1.53
2	A	900	ADX	C2'-C3'	-2.26	1.47	1.53
2	B	900	ADX	C1'-N9	-2.23	1.40	1.46
2	D	900	ADX	C3'-C4'	-2.20	1.47	1.53
2	F	900	ADX	C5-N7	-2.19	1.35	1.39
2	G	900	ADX	C5-N7	-2.19	1.35	1.39
2	D	900	ADX	C2'-C3'	-2.15	1.47	1.53
2	D	900	ADX	C5-N7	-2.14	1.35	1.39
2	F	900	ADX	C2'-C3'	-2.13	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	ADX	C2'-C3'	-2.13	1.47	1.53
2	E	900	ADX	C1'-N9	-2.12	1.40	1.46
2	B	900	ADX	C2'-C3'	-2.11	1.47	1.53
2	A	900	ADX	C3'-C4'	-2.06	1.47	1.53
2	H	900	ADX	C3'-C4'	-2.01	1.47	1.53

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	ADX	C5-C4-N3	-5.75	118.81	126.72
2	G	900	ADX	C5-C4-N3	-5.38	119.31	126.72
2	H	900	ADX	C5-C4-N3	-5.31	119.41	126.72
2	B	900	ADX	C5-C4-N3	-5.20	119.56	126.72
2	A	900	ADX	C5-C4-N3	-5.07	119.73	126.72
2	E	900	ADX	C5-C4-N3	-5.00	119.83	126.72
2	F	900	ADX	C5-C4-N3	-4.94	119.91	126.72
2	D	900	ADX	C5-C4-N3	-4.93	119.92	126.72
2	C	900	ADX	N9-C8-N7	-4.77	107.17	113.94
2	C	900	ADX	N3-C2-N1	-4.72	121.43	128.58
2	H	900	ADX	N3-C2-N1	-4.70	121.47	128.58
2	B	900	ADX	N3-C2-N1	-4.63	121.57	128.58
2	G	900	ADX	N3-C4-N9	4.61	135.00	127.17
2	F	900	ADX	N3-C2-N1	-4.60	121.62	128.58
2	A	900	ADX	N3-C2-N1	-4.59	121.64	128.58
2	C	900	ADX	N3-C4-N9	4.51	134.83	127.17
2	G	900	ADX	N9-C8-N7	-4.47	107.59	113.94
2	B	900	ADX	N9-C8-N7	-4.41	107.67	113.94
2	G	900	ADX	C4-N9-C8	4.36	110.32	105.74
2	A	900	ADX	N9-C8-N7	-4.29	107.85	113.94
2	H	900	ADX	N9-C8-N7	-4.25	107.90	113.94
2	B	900	ADX	N3-C4-N9	4.23	134.37	127.17
2	D	900	ADX	N3-C2-N1	-4.23	122.17	128.58
2	H	900	ADX	N3-C4-N9	4.15	134.23	127.17
2	F	900	ADX	N9-C8-N7	-4.14	108.06	113.94
2	E	900	ADX	N3-C2-N1	-4.08	122.41	128.58
2	C	900	ADX	C5-N7-C8	4.08	109.86	103.45
2	A	900	ADX	N3-C4-N9	4.08	134.10	127.17
2	B	900	ADX	C4-N9-C8	4.04	109.98	105.74
2	E	900	ADX	N9-C8-N7	-4.02	108.24	113.94
2	G	900	ADX	N3-C2-N1	-3.99	122.54	128.58
2	B	900	ADX	O5'-PA-O3A	3.91	114.94	103.09
2	A	900	ADX	C4-N9-C8	3.91	109.84	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	900	ADX	N3-C4-N9	3.86	133.74	127.17
2	H	900	ADX	C4-N9-C8	3.81	109.74	105.74
2	C	900	ADX	C4-N9-C8	3.74	109.67	105.74
2	C	900	ADX	C2-N3-C4	3.71	120.90	111.83
2	H	900	ADX	C5-N7-C8	3.69	109.26	103.45
2	F	900	ADX	C4-N9-C8	3.68	109.60	105.74
2	D	900	ADX	N3-C4-N9	3.68	133.42	127.17
2	E	900	ADX	N3-C4-N9	3.61	133.31	127.17
2	B	900	ADX	C5-N7-C8	3.58	109.08	103.45
2	G	900	ADX	C5-N7-C8	3.55	109.04	103.45
2	B	900	ADX	C2-N3-C4	3.55	120.49	111.83
2	A	900	ADX	C5-N7-C8	3.50	108.96	103.45
2	H	900	ADX	C2-N3-C4	3.49	120.36	111.83
2	D	900	ADX	N9-C8-N7	-3.48	109.00	113.94
2	E	900	ADX	C4-N9-C8	3.48	109.39	105.74
2	A	900	ADX	C2-N3-C4	3.39	120.11	111.83
2	H	900	ADX	C4-C5-N7	-3.36	106.74	110.58
2	E	900	ADX	C5-N7-C8	3.35	108.71	103.45
2	E	900	ADX	C4-C5-N7	-3.31	106.80	110.58
2	F	900	ADX	C2-N3-C4	3.30	119.90	111.83
2	F	900	ADX	C5-N7-C8	3.30	108.64	103.45
2	D	900	ADX	C5-N7-C8	3.29	108.62	103.45
2	G	900	ADX	C2-N3-C4	3.23	119.72	111.83
2	G	900	ADX	O5'-PA-O3A	3.20	112.78	103.09
2	C	900	ADX	C4-C5-N7	-3.19	106.94	110.58
2	D	900	ADX	C2-N3-C4	3.15	119.52	111.83
2	E	900	ADX	C2-N3-C4	3.10	119.40	111.83
2	D	900	ADX	C4-C5-N7	-3.06	107.08	110.58
2	B	900	ADX	C4-C5-N7	-2.98	107.17	110.58
2	A	900	ADX	C4-C5-N7	-2.98	107.18	110.58
2	F	900	ADX	C4-C5-N7	-2.84	107.33	110.58
2	E	900	ADX	O5'-PA-O3A	2.83	111.66	103.09
2	G	900	ADX	C4-C5-N7	-2.81	107.37	110.58
2	D	900	ADX	C4-N9-C8	2.75	108.62	105.74
2	A	900	ADX	O5'-PA-O3A	2.71	111.29	103.09
2	D	900	ADX	O5'-PA-O3A	2.41	110.40	103.09
2	C	900	ADX	O5'-C5'-C4'	2.26	116.67	108.99
2	E	900	ADX	C4-N9-C1'	-2.23	121.42	126.63
2	B	900	ADX	O5'-C5'-C4'	2.21	116.51	108.99
2	F	900	ADX	O5'-PA-O3A	2.17	109.66	103.09
2	E	900	ADX	O5'-C5'-C4'	2.17	116.37	108.99
2	D	900	ADX	C4-N9-C1'	-2.11	121.70	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	ADX	O4'-C1'-N9	-2.09	104.08	108.09
2	D	900	ADX	O5'-C5'-C4'	2.08	116.06	108.99
2	H	900	ADX	O5'-C5'-C4'	2.03	115.90	108.99

There are no chirality outliers.

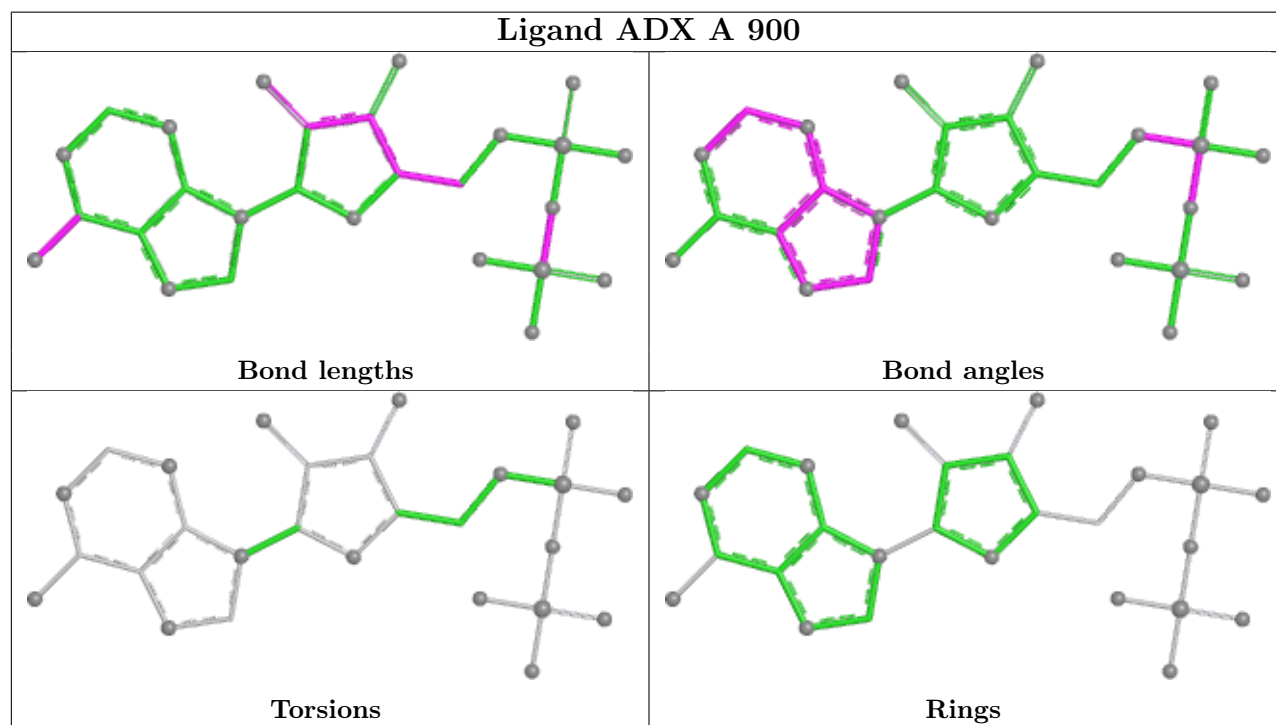
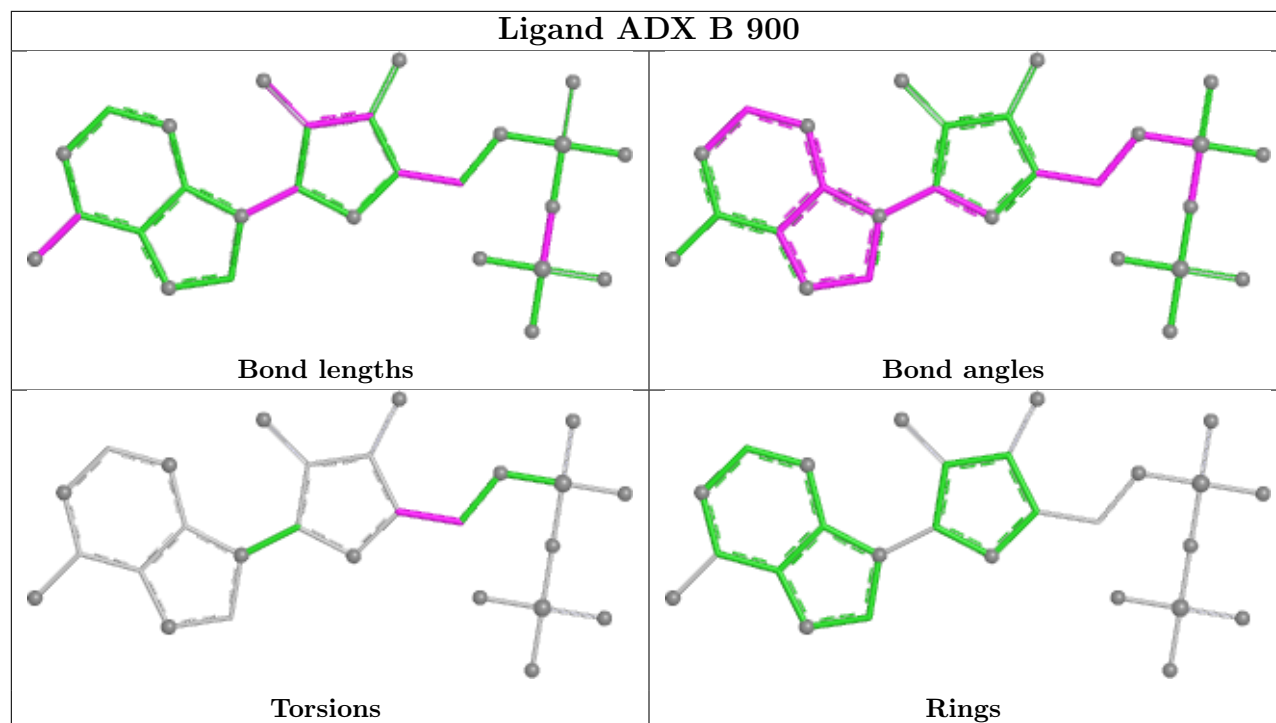
All (12) torsion outliers are listed below:

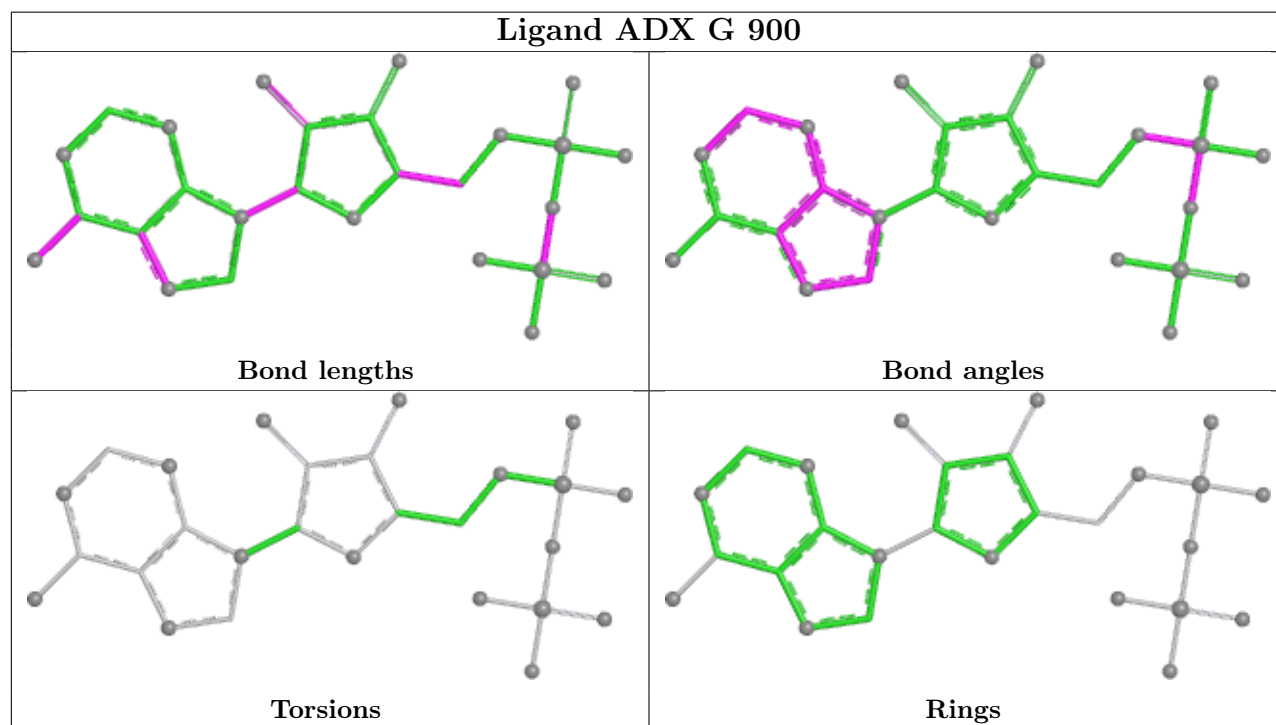
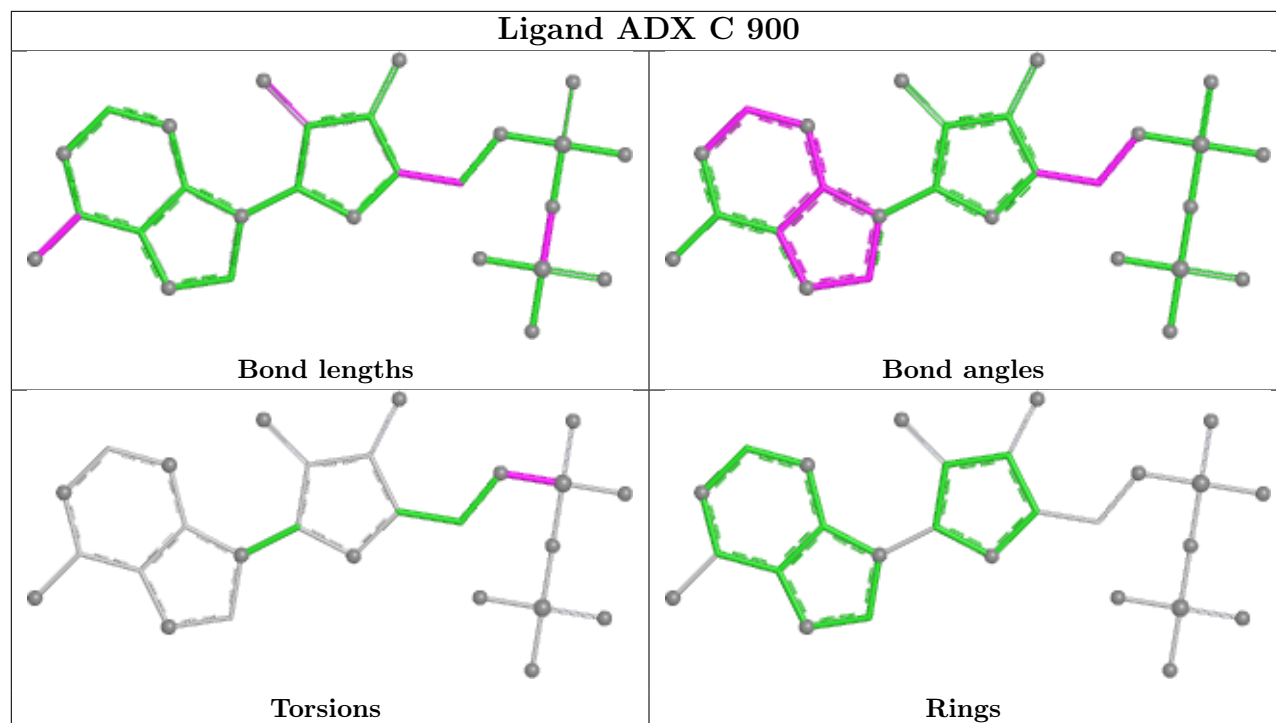
Mol	Chain	Res	Type	Atoms
2	C	900	ADX	C5'-O5'-PA-O1A
2	F	900	ADX	C5'-O5'-PA-O1A
2	F	900	ADX	C5'-O5'-PA-O3A
2	H	900	ADX	C5'-O5'-PA-O1A
2	H	900	ADX	C5'-O5'-PA-O2A
2	H	900	ADX	C5'-O5'-PA-O3A
2	C	900	ADX	C5'-O5'-PA-O2A
2	C	900	ADX	C5'-O5'-PA-O3A
2	D	900	ADX	C5'-O5'-PA-O2A
2	E	900	ADX	C5'-O5'-PA-O3A
2	F	900	ADX	C5'-O5'-PA-O2A
2	B	900	ADX	O4'-C4'-C5'-O5'

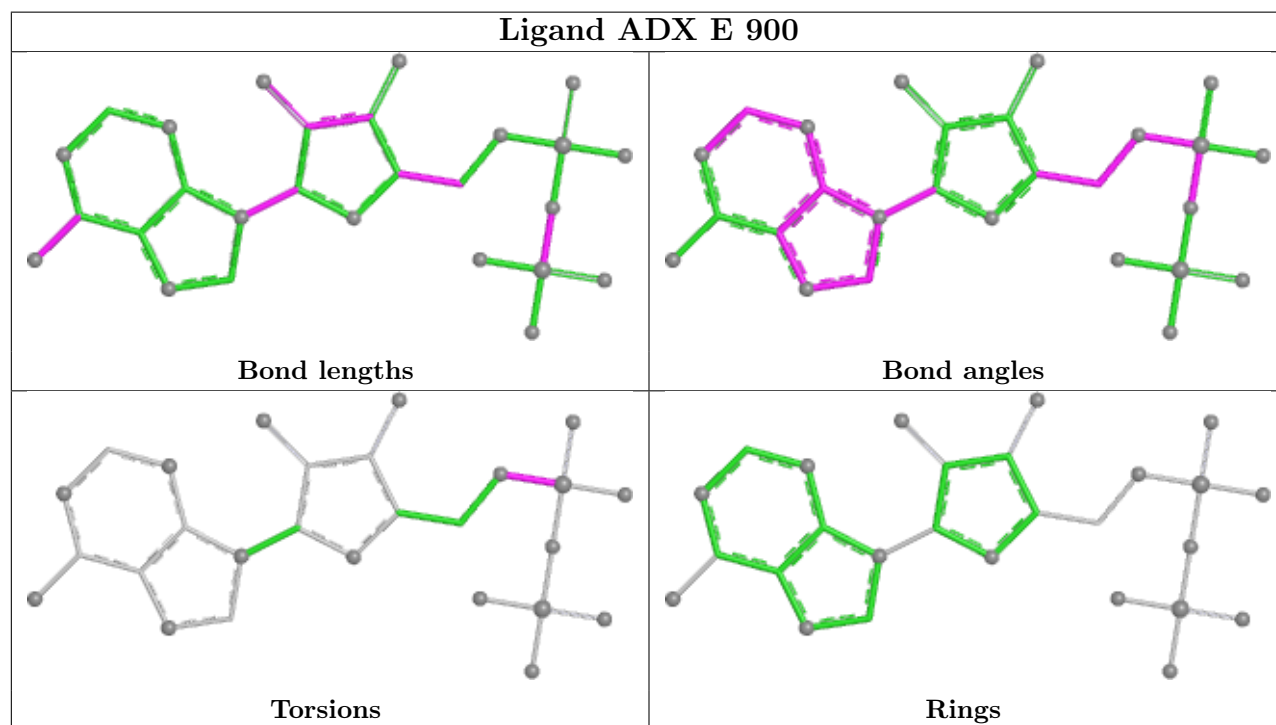
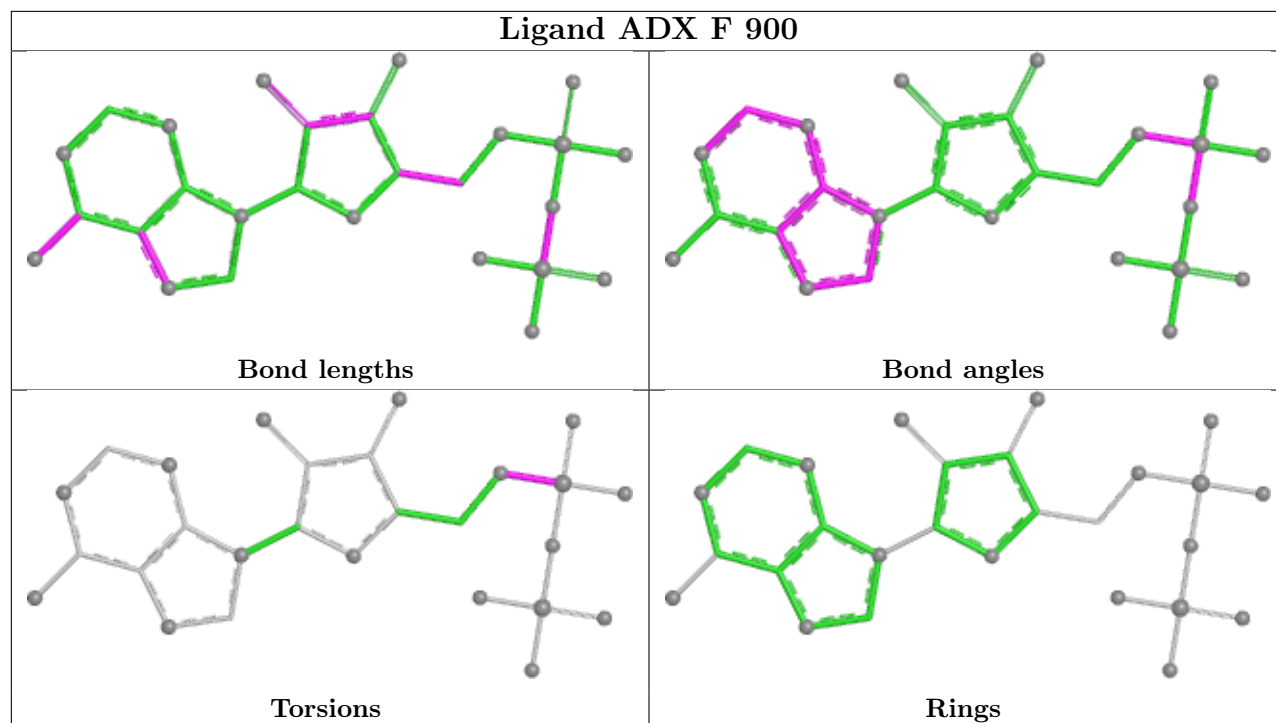
There are no ring outliers.

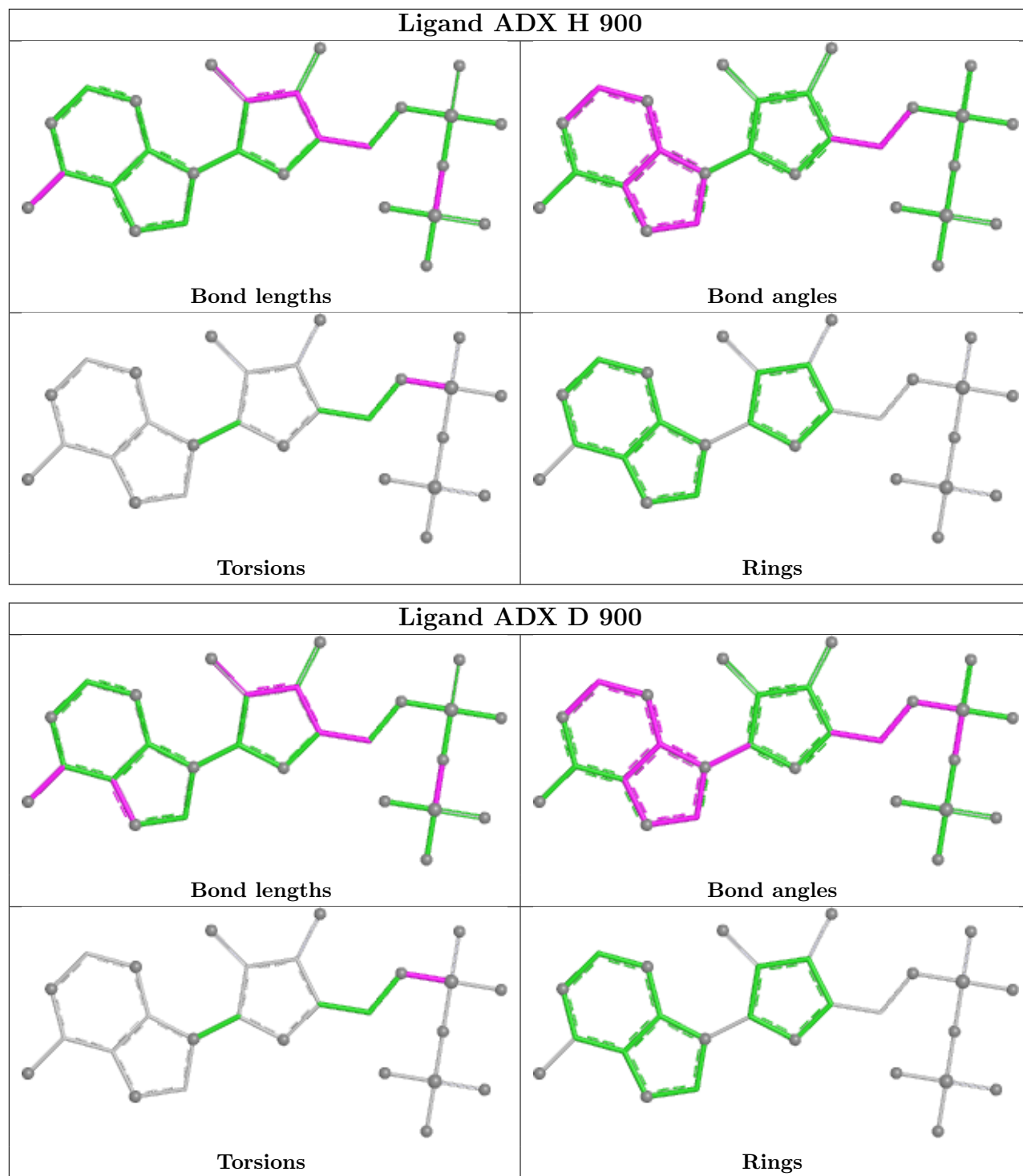
No monomer is involved in short contacts.

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	402/404 (99%)	-0.11	4 (0%) 79 77	29, 47, 76, 106	0
1	B	404/404 (100%)	-0.38	1 (0%) 91 90	18, 39, 68, 103	2 (0%)
1	C	403/404 (99%)	-0.57	1 (0%) 91 90	16, 30, 56, 70	0
1	D	401/404 (99%)	-0.20	4 (0%) 79 77	21, 43, 76, 110	0
1	E	403/404 (99%)	0.00	8 (1%) 65 62	19, 37, 68, 99	0
1	F	401/404 (99%)	-0.01	3 (0%) 84 82	31, 53, 82, 104	0
1	G	404/404 (100%)	0.14	6 (1%) 72 69	24, 39, 71, 108	0
1	H	381/404 (94%)	0.79	30 (7%) 18 16	47, 84, 117, 146	0
All	All	3199/3232 (98%)	-0.05	57 (1%) 67 65	16, 44, 91, 146	2 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	155	ASP	4.5
1	H	445	TYR	4.1
1	D	65	PHE	4.0
1	G	65	PHE	4.0
1	H	429	PRO	4.0
1	H	214	ILE	3.3
1	G	69	LEU	3.2
1	D	155	ASP	3.2
1	H	199	ALA	3.1
1	H	69	LEU	3.1
1	H	158	GLY	3.1
1	E	65	PHE	3.0
1	B	65	PHE	2.9
1	E	69	LEU	2.9
1	H	287	ALA	2.8
1	D	143	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	154	PHE	2.7
1	H	216	TYR	2.7
1	H	411	LEU	2.6
1	H	143	HIS	2.6
1	F	122	ASP	2.6
1	C	48	MET	2.6
1	H	219	GLY	2.6
1	G	137	ILE	2.6
1	H	441	LEU	2.5
1	A	65	PHE	2.5
1	F	448	LEU	2.4
1	H	65	PHE	2.4
1	E	158	GLY	2.4
1	H	55	GLY	2.4
1	D	48	MET	2.4
1	H	315	VAL	2.3
1	E	138	ASP	2.3
1	A	48	MET	2.3
1	H	68	ASP	2.3
1	H	157	LYS	2.3
1	H	160	PRO	2.3
1	E	268	GLU	2.2
1	H	290	VAL	2.2
1	E	156	SER	2.2
1	G	67	ARG	2.2
1	H	391	ALA	2.2
1	H	438	TRP	2.2
1	H	442	VAL	2.1
1	H	435	PRO	2.1
1	H	223	PHE	2.1
1	H	251	VAL	2.1
1	H	238	ASN	2.1
1	H	200	GLY	2.1
1	H	220	LEU	2.1
1	F	445	TYR	2.1
1	A	360	LYS	2.1
1	A	449	VAL	2.1
1	H	212	GLU	2.1
1	G	63	THR	2.0
1	H	154	PHE	2.0
1	E	48	MET	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](#)

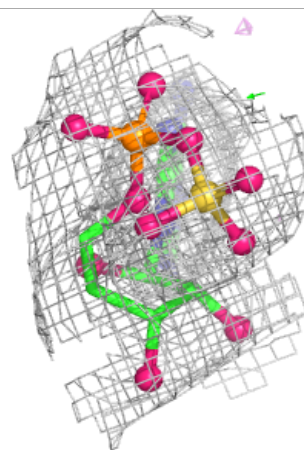
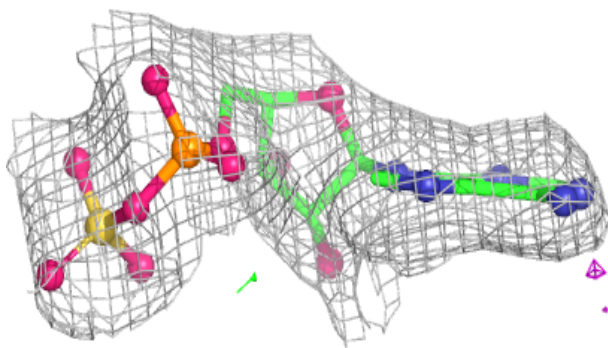
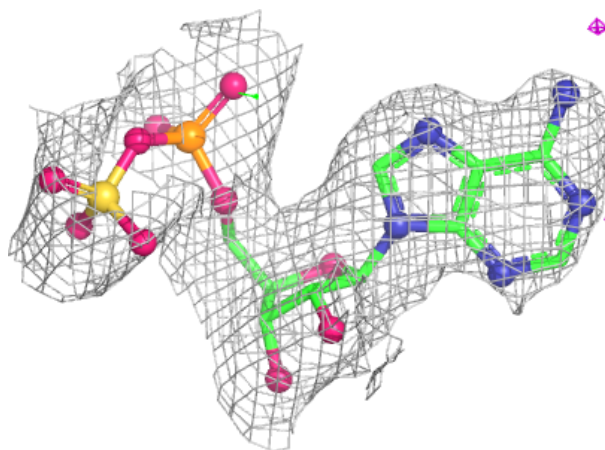
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	ADX	H	900	27/27	0.94	0.10	71,78,84,91	0
2	ADX	G	900	27/27	0.97	0.06	20,27,33,35	0
2	ADX	F	900	27/27	0.97	0.07	39,48,53,56	0
2	ADX	B	900	27/27	0.98	0.05	22,29,34,38	0
2	ADX	D	900	27/27	0.98	0.05	21,28,30,32	0
2	ADX	E	900	27/27	0.98	0.06	21,29,34,37	0
2	ADX	C	900	27/27	0.99	0.05	17,23,30,32	0
2	ADX	A	900	27/27	0.99	0.04	27,32,36,38	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.

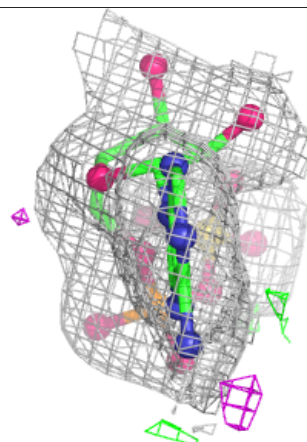
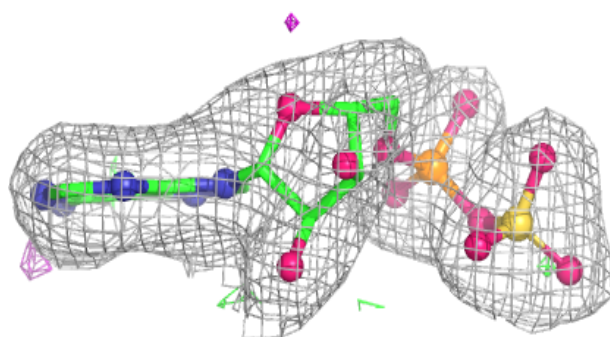
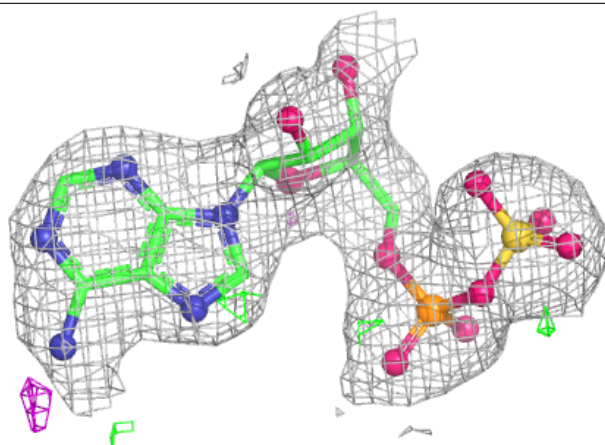
Electron density around ADX H 900:

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



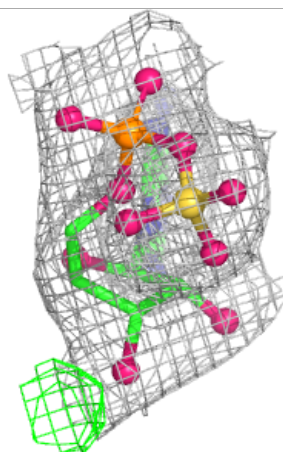
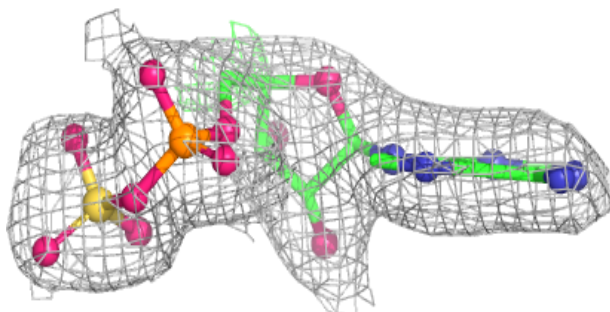
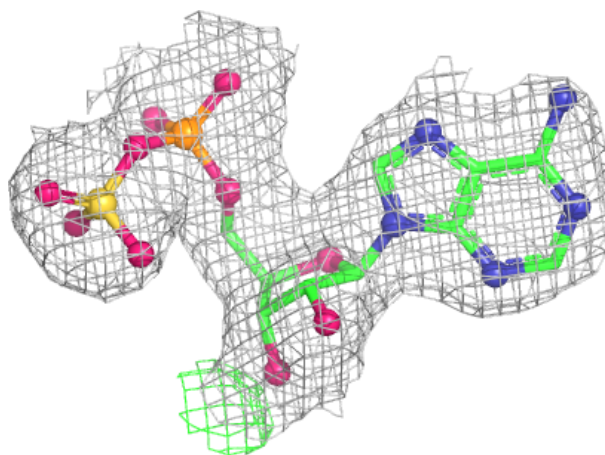
Electron density around ADX G 900:

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



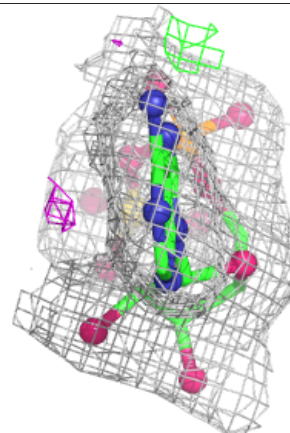
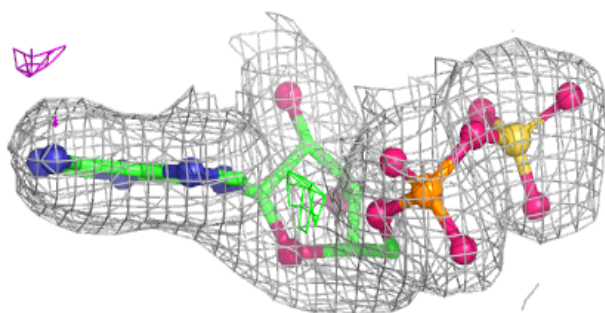
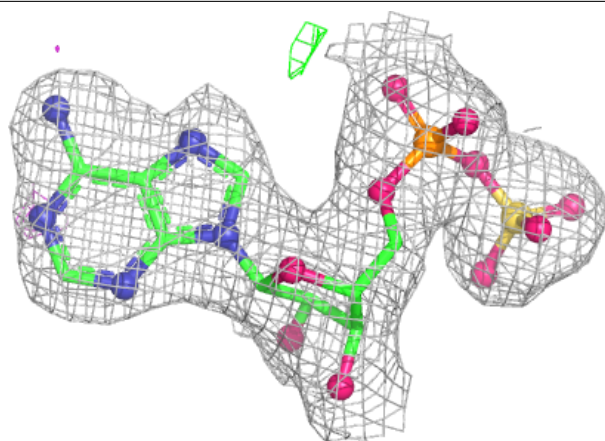
Electron density around ADX F 900:

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



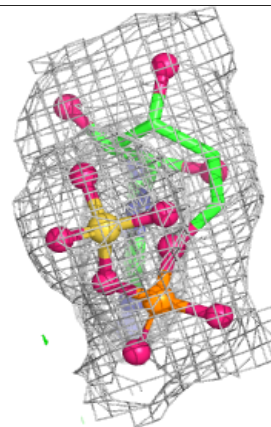
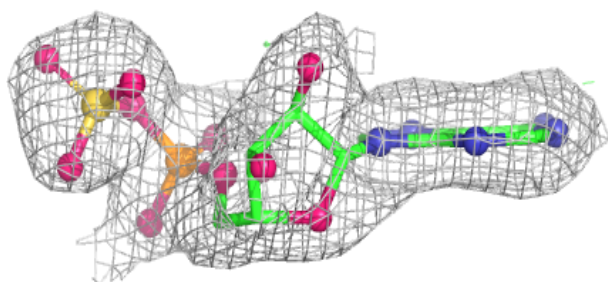
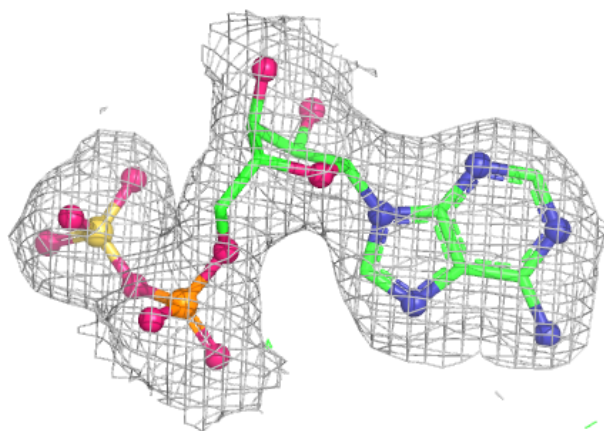
Electron density around ADX B 900:

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



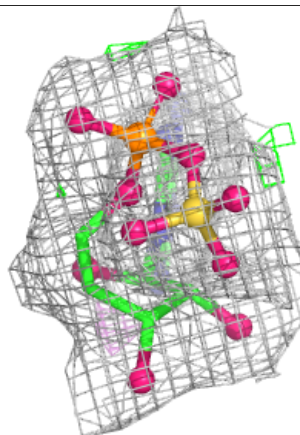
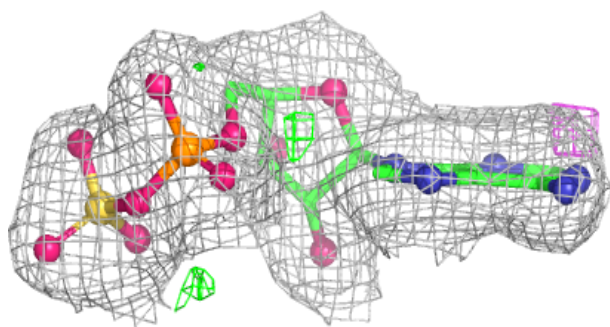
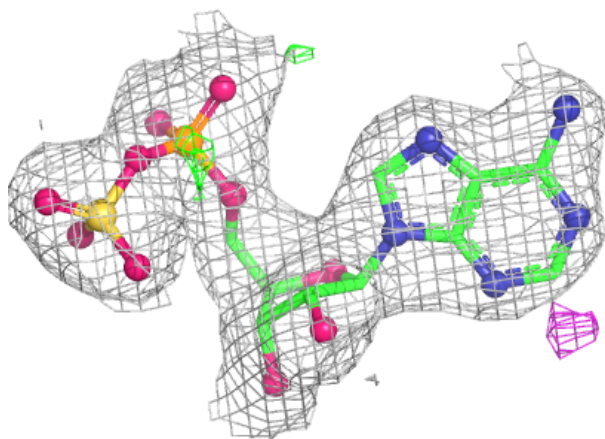
Electron density around ADX D 900:

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



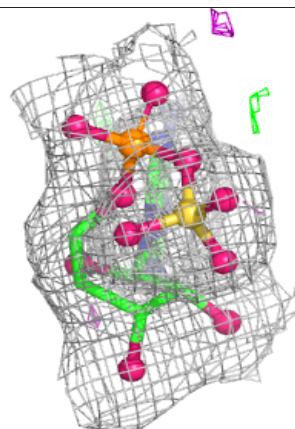
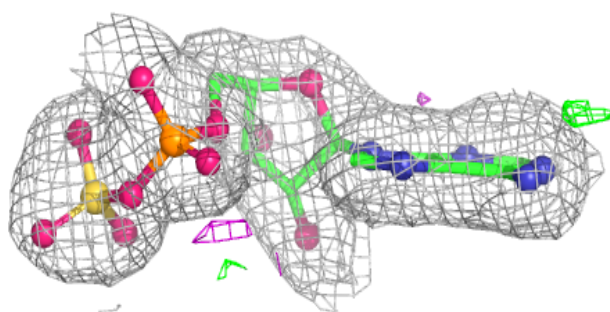
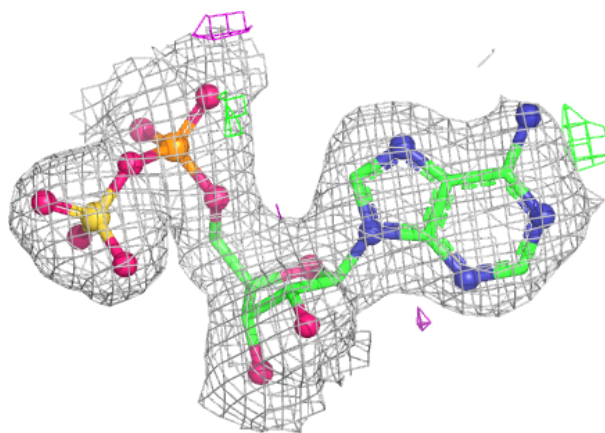
Electron density around ADX E 900:

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



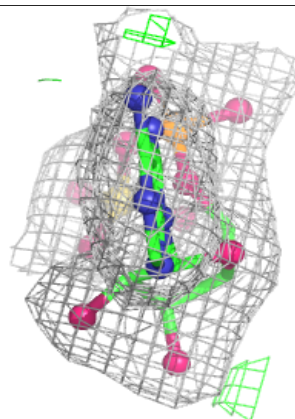
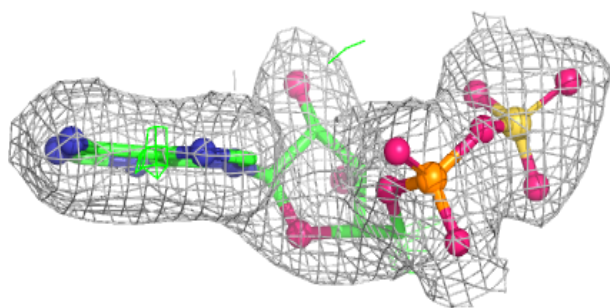
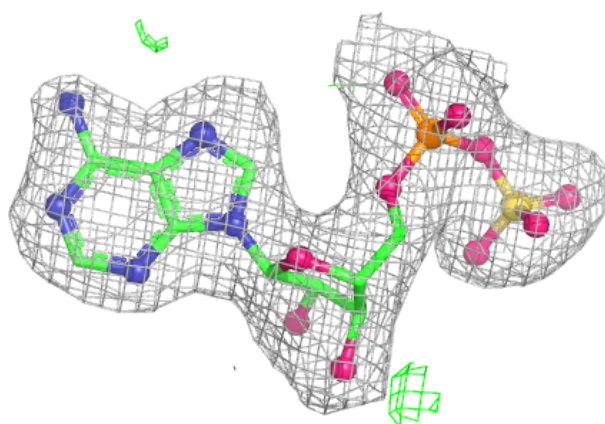
Electron density around ADX C 900:

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



Electron density around ADX A 900:

$2mF_o-DF_c$ (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.