



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:17 PM BST

PDB ID : 4MAF
Title : Soybean ATP Sulfurylase
Authors : Herrmann, J.; Ravilious, G.E.; McKinney, S.E.; Westfall, C.S.; Lee, S.G.;
Krishnan, H.B.; Jez, J.M.
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

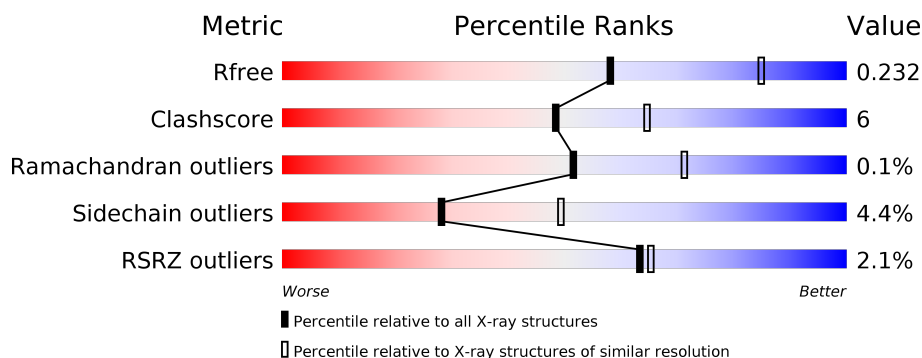
1 Overall quality at a glance

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}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	404	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
1	B	404	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>14%</div> <div></div> </div> </div>
1	C	404	<div> <div></div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
1	D	404	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
1	E	404	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>
1	F	404	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	404	<div><div>%</div><div><div></div><div>84%</div><div>15%</div><div></div></div><div></div></div>
1	H	404	<div><div>8%</div><div><div></div><div>72%</div><div>21%</div><div>6%</div></div><div></div></div>

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:

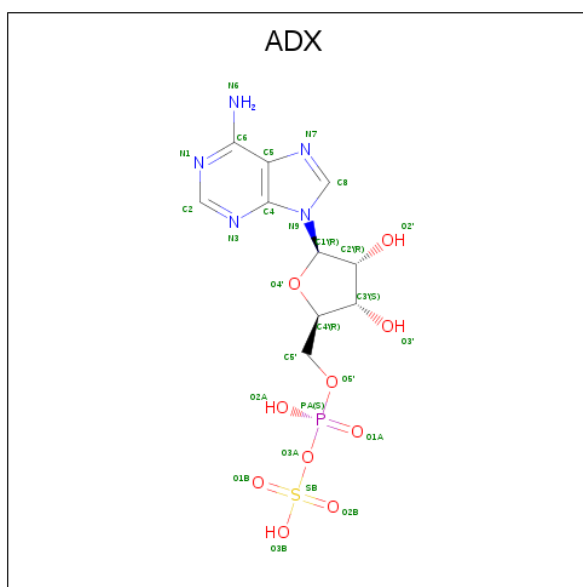
Chain	Residue	Modelled	Actual	Comment	Reference
A	48	MET	-	INITIATING METHIONINE	UNP Q8SAG1
A	450	LEU	-	EXPRESSION TAG	UNP Q8SAG1
A	451	SER	-	EXPRESSION TAG	UNP Q8SAG1
B	48	MET	-	INITIATING METHIONINE	UNP Q8SAG1
B	450	LEU	-	EXPRESSION TAG	UNP Q8SAG1
B	451	SER	-	EXPRESSION TAG	UNP Q8SAG1
C	48	MET	-	INITIATING 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

Continued on next page...

Continued from previous page...

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 (three-letter code: ADX) (formula: $C_{10}H_{14}N_5O_{10}PS$).



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

Continued on next page...

Continued from previous page...

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

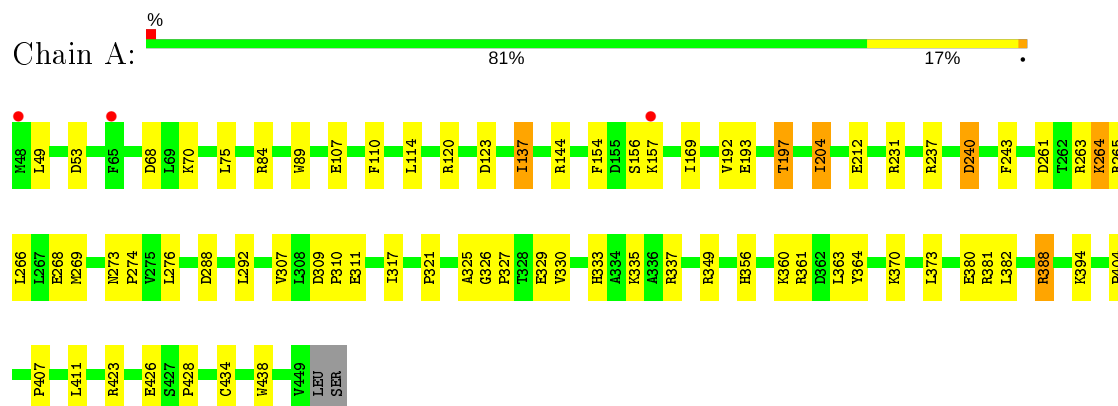
- Molecule 3 is water.

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

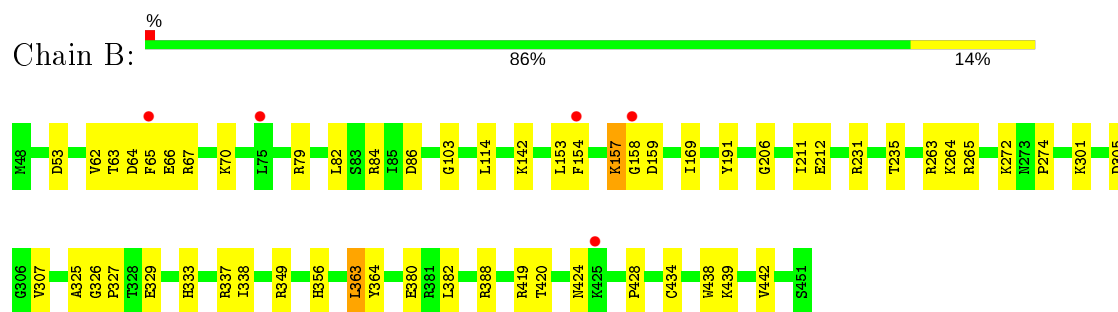
3 Residue-property plots [i](#)

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.

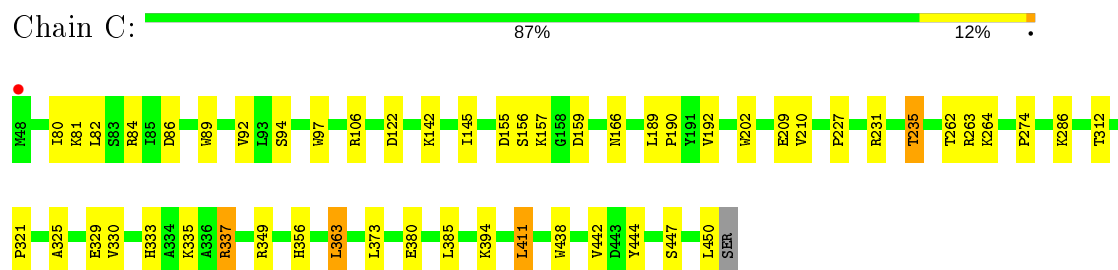
• Molecule 1: ATP sulfurylase



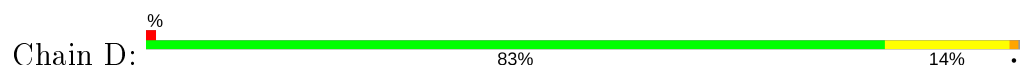
• Molecule 1: ATP sulfurylase

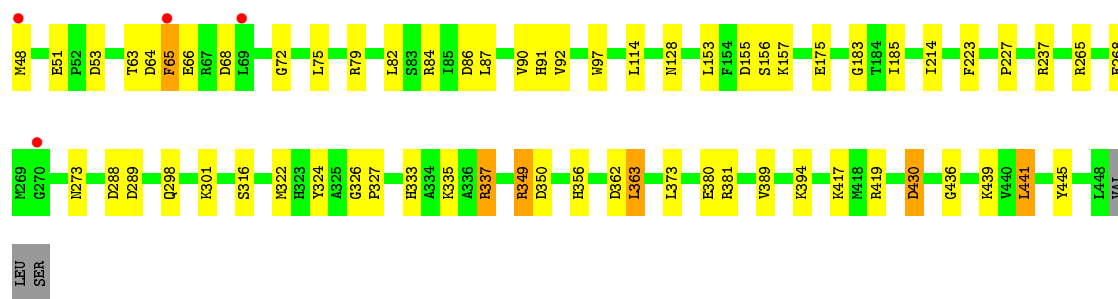


• Molecule 1: ATP sulfurylase

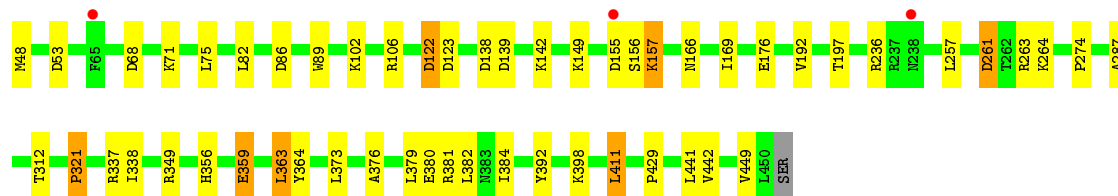
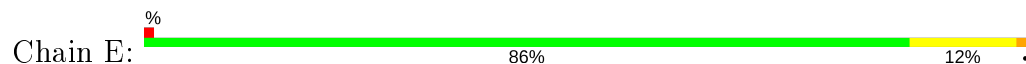


• Molecule 1: ATP sulfurylase

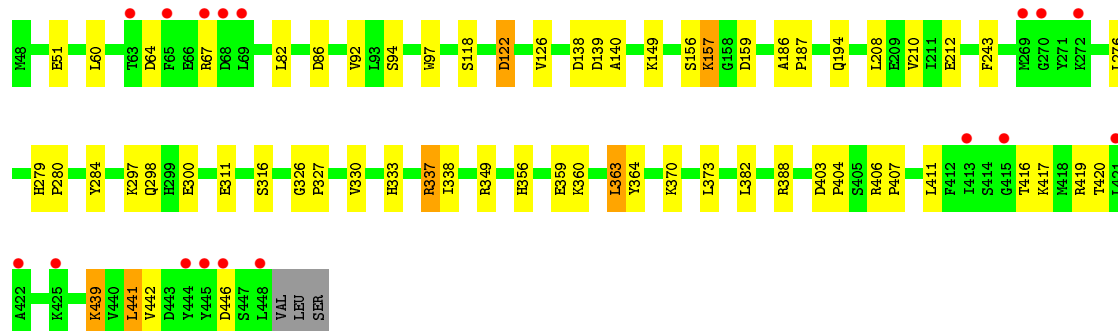
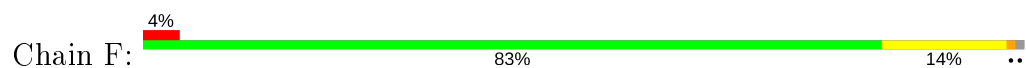




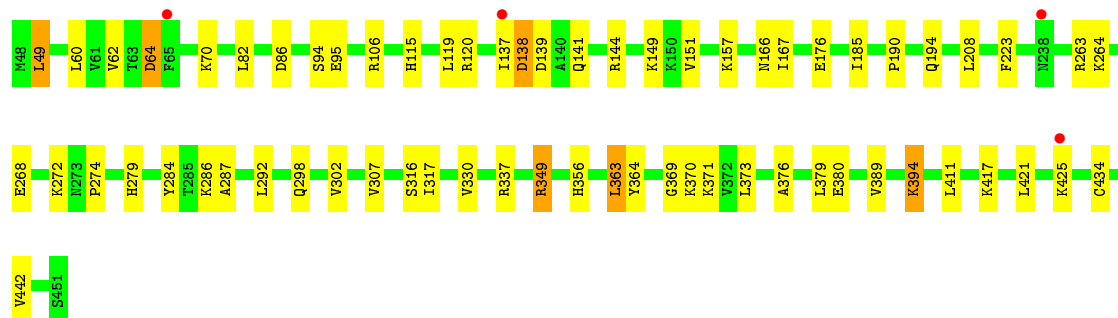
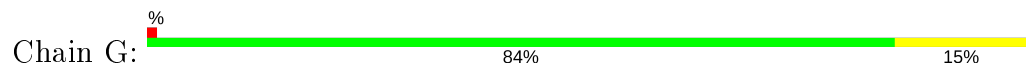
- Molecule 1: ATP sulfurylase



- 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 48.55 – 2.48	Depositor EDS
% Data completeness (in resolution range)	93.5 (48.21-2.48) 88.6 (48.55-2.48)	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 0.185 , 0.232	Depositor DCC
R_{free} test set	6239 reflections (5.05%)	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)	0.31 , 48.2	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	0.37	0/3278	0.56	0/4447
1	B	0.39	0/3306	0.57	0/4485
1	C	0.44	0/3286	0.59	0/4458
1	D	0.42	0/3271	0.58	0/4437
1	E	0.42	0/3286	0.59	0/4458
1	F	0.35	0/3271	0.54	0/4437
1	G	0.42	0/3292	0.57	0/4466
1	H	0.30	0/3116	0.51	0/4228
All	All	0.39	0/26106	0.56	0/35416

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.

There are no bond angle outliers.

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	47	0
1	B	3219	0	3215	33	0
1	C	3205	0	3201	33	0
1	D	3190	0	3181	37	0
1	E	3205	0	3201	34	0
1	F	3190	0	3181	33	0
1	G	3211	0	3206	41	0
1	H	3037	0	3018	57	0
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	3	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	306	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 (306) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:297:LYS:NZ	3:H:1020:HOH:O	2.18	0.77
1:B:63:THR:OG1	1:B:66:GLU:OE2	2.03	0.76
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:A:266:LEU:HD23	1:A:269:MET:HE3	1.73	0.70
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
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:H:291:PRO:HG2	1:H:294:TRP:HD1	1.60	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:OD1	1:H:123:ASP:N	2.29	0.66
1:A:237:ARG:NH1	1:A:311:GLU:O	2.28	0.65
1:A:240:ASP:OD1	1:A:240:ASP:N	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:155:ASP:CG	1:E:156:SER:HB3	2.21	0.61
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:A:360:LYS:HE2	3:A:1065:HOH:O	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:301:LYS:HE2	1:B:439:LYS:HZ1	1.66	0.59
1:D:265:ARG:HB2	1:D:265:ARG:HH11	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
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: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:H:294:TRP:CE3	1:H:444:TYR:HB2	2.40	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: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: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:F:360:LYS:HA	1:F:360:LYS:HZ2	1.71	0.53
1:H:67:ARG:HG3	1:H:211:ILE:HG23	1.89	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:NH2	3:A:1044:HOH:O	2.41	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
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: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:B:191:TYR:OH	3:B:1052:HOH:O	2.16	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: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:N	1:D:430:ASP:OD2	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:E:192:VAL:HG12	1:E:197:THR:HG23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:TRP:CZ2	1:C:321:PRO:HG2	2.49	0.48
1:G:330:VAL:HG13	1:G:373:LEU:HD13	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
3:A:1050:HOH:O	1:H:115:HIS:HD2	1.95	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:G:380:GLU:H	1:G:380:GLU:CD	2.17	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:D:316:SER:OG	3:D:1012:HOH:O	2.15	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:B:301:LYS:CE	1:B:439:LYS:HZ1	2.28	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: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: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:A:380:GLU:HG2	1:H:120:ARG:NH2	2.30	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:243:PHE:CZ	1:F:276:LEU:HB2	2.51	0.46
1:C:380:GLU:H	1:C:380:GLU:CD	2.20	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: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:439:LYS:O	1:F:442:VAL:HG22	2.17	0.45
1:F:92:VAL:HG13	1:F:97:TRP:HB2	1.99	0.45
1:G:425:LYS:HB3	1:G:425:LYS:HE2	1.56	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:HA	1:H:185:ILE:HD13	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:E:380:GLU:CD	1:E:380:GLU:H	2.21	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:C:444:TYR:O	1:C:447:SER:HB2	2.18	0.44
1:G:185:ILE:HD13	1:G:185:ILE:HA	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:N	1:E:122:ASP:OD2	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:130:SER:N	3:H:1005:HOH:O	2.37	0.44
1:H:49:LEU:HD12	1:H:50:ILE:H	1.83	0.44
1:A:107:GLU:OE1	1:H:371:LYS:NZ	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:LYS:HD2	1:E:169:ILE:HG21	1.98	0.43
1:D:75:LEU:HD11	1:H:75:LEU:HD11	1.99	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: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:H:307:VAL:HG21	1:H:434:CYS:HB3	2.01	0.42
1:H:95:GLU:HB3	1:H:227:PRO:HD2	2.00	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:HA	1:C:411:LEU:HD12	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:HA	1:G:137:ILE:HD13	1.79	0.42
1:G:363:LEU:HB3	1:G:364:TYR:CD2	2.54	0.42
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	1:A:265:ARG:HE	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:194:GLN:HG3	1:F:284:TYR:CZ	2.55	0.41
1:F:94:SER:HB3	1:F:210:VAL:HG21	2.01	0.41
1:H:153:LEU:O	1:H:161:VAL:HG22	2.20	0.41
1:B:380:GLU:H	1:B:380:GLU:CD	2.24	0.41
1:F:411:LEU:HD12	1:F:411:LEU:HA	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:HD3	1:G:70:LYS:HA	1.85	0.41
1:D:373:LEU:HD12	1:D:373:LEU:HA	1.90	0.41
1:D:92:VAL:HG13	1:D:97:TRP:HB2	2.03	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:388:ARG:HG2	1:A:388:ARG:H	1.69	0.41
1:A:75:LEU:HD23	1:A:154:PHE:HZ	1.86	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: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:B:103:GLY:HA3	1:B:206:GLY:O	2.21	0.41
1:B:380:GLU:OE1	3:B:1088:HOH:O	2.21	0.41
1:F:419:ARG:HG3	1:F:419:ARG:HH11	1.86	0.41
1:G:138:ASP:HB2	1:G:141:GLN:OE1	2.20	0.41
1:G:60:LEU:HB2	1:G:94:SER:HA	2.01	0.41
1:H:291:PRO:HG2	1:H:294:TRP:CD1	2.48	0.41
1:A:120:ARG:NH2	1:H:375:MET:O	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:THR:O	1:B:424:ASN:ND2	2.50	0.41
1:C:262:THR:HG23	1:C:385:LEU:HD13	2.03	0.41
1:D:394:LYS:HB2	1:D:394:LYS:HE3	1.71	0.41
1:H:56:LYS:HA	1:H:56:LYS:HD3	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:N	1:E:123:ASP:OD1	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:393:ASP:OD2	1:H:396:GLN:NE2	2.52	0.40
1:H:91:HIS:NE2	1:H:95:GLU:OE2	2.53	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%)	29	46
1	C	401/404 (99%)	396 (99%)	5 (1%)	0	100	100
1	D	399/404 (99%)	388 (97%)	10 (2%)	1 (0%)	41	59
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	377/404 (93%)	360 (96%)	16 (4%)	1 (0%)	41	59
All	All	3183/3232 (98%)	3113 (98%)	66 (2%)	4 (0%)	51	71

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%)	28	49
1	B	348/346 (101%)	336 (97%)	12 (3%)	37	61
1	C	345/346 (100%)	337 (98%)	8 (2%)	50	74
1	D	343/346 (99%)	325 (95%)	18 (5%)	23	41
1	E	345/346 (100%)	326 (94%)	19 (6%)	21	39
1	F	343/346 (99%)	326 (95%)	17 (5%)	24	43
1	G	346/346 (100%)	330 (95%)	16 (5%)	27	47
1	H	325/346 (94%)	309 (95%)	16 (5%)	25	44
All	All	2739/2768 (99%)	2618 (96%)	121 (4%)	28	49

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASP
1	A	84	ARG
1	A	123	ASP
1	A	137	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	349	ARG
1	A	388	ARG
1	A	426	GLU
1	B	53[A]	ASP
1	B	53[B]	ASP
1	B	64	ASP
1	B	65	PHE
1	B	84	ARG
1	B	114	LEU
1	B	212	GLU
1	B	272	LYS
1	B	305	ASP
1	B	349	ARG
1	B	363	LEU
1	B	419	ARG
1	C	84	ARG
1	C	235	THR
1	C	335	LYS
1	C	337	ARG
1	C	349	ARG
1	C	363	LEU
1	C	411	LEU
1	C	450	LEU
1	D	48	MET
1	D	51	GLU
1	D	64	ASP
1	D	65	PHE
1	D	79	ARG
1	D	84	ARG
1	D	87	LEU
1	D	114	LEU
1	D	223	PHE
1	D	268	GLU
1	D	288	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	335	LYS
1	D	337	ARG
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	122	ASP
1	E	138	ASP
1	E	139	ASP
1	E	157	LYS
1	E	236	ARG
1	E	261	ASP
1	E	321	PRO
1	E	337	ARG
1	E	349	ARG
1	E	359	GLU
1	E	363	LEU
1	E	398	LYS
1	E	411	LEU
1	E	441	LEU
1	E	442	VAL
1	E	449	VAL
1	F	51	GLU
1	F	122	ASP
1	F	139	ASP
1	F	149	LYS
1	F	156	SER
1	F	157	LYS
1	F	297	LYS
1	F	300	GLU
1	F	311	GLU
1	F	337	ARG
1	F	349	ARG
1	F	359	GLU
1	F	363	LEU
1	F	388	ARG
1	F	439	LYS
1	F	441	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	446	ASP
1	G	49	LEU
1	G	64	ASP
1	G	120	ARG
1	G	138	ASP
1	G	139	ASP
1	G	149	LYS
1	G	157	LYS
1	G	264	LYS
1	G	268	GLU
1	G	272	LYS
1	G	337	ARG
1	G	349	ARG
1	G	363	LEU
1	G	370	LYS
1	G	394	LYS
1	G	442	VAL
1	H	63	THR
1	H	122	ASP
1	H	123	ASP
1	H	138	ASP
1	H	212	GLU
1	H	228	THR
1	H	261	ASP
1	H	263	ARG
1	H	264	LYS
1	H	272	LYS
1	H	273	ASN
1	H	279	HIS
1	H	301	LYS
1	H	337	ARG
1	H	349	ARG
1	H	381	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	323	HIS
1	H	115	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	900	-	25,29,29	1.69	7 (28%)	26,45,45	1.42	4 (15%)
2	ADX	C	900	-	25,29,29	1.52	4 (16%)	26,45,45	1.40	5 (19%)
2	ADX	E	900	-	25,29,29	1.53	5 (20%)	26,45,45	1.43	5 (19%)
2	ADX	B	900	-	25,29,29	1.54	5 (20%)	26,45,45	1.50	5 (19%)
2	ADX	G	900	-	25,29,29	1.60	5 (20%)	26,45,45	1.38	2 (7%)
2	ADX	D	900	-	25,29,29	1.64	7 (28%)	26,45,45	1.48	5 (19%)
2	ADX	F	900	-	25,29,29	1.73	7 (28%)	26,45,45	1.37	3 (11%)
2	ADX	H	900	-	25,29,29	1.65	6 (24%)	26,45,45	1.41	4 (15%)

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	A	900	-	-	0/6/32/32	0/3/3/3
2	ADX	C	900	-	-	3/6/32/32	0/3/3/3
2	ADX	E	900	-	-	2/6/32/32	0/3/3/3
2	ADX	B	900	-	-	1/6/32/32	0/3/3/3
2	ADX	G	900	-	-	0/6/32/32	0/3/3/3
2	ADX	D	900	-	-	1/6/32/32	0/3/3/3
2	ADX	F	900	-	-	3/6/32/32	0/3/3/3
2	ADX	H	900	-	-	3/6/32/32	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	900	ADX	C2'-C1'	-4.09	1.47	1.53
2	G	900	ADX	C2'-C1'	-3.98	1.47	1.53
2	A	900	ADX	C2'-C1'	-3.65	1.48	1.53
2	H	900	ADX	C2'-C1'	-3.61	1.48	1.53
2	B	900	ADX	C2'-C1'	-3.46	1.48	1.53
2	H	900	ADX	O2'-C2'	-3.46	1.34	1.43
2	F	900	ADX	O2'-C2'	-3.43	1.34	1.43
2	C	900	ADX	C2'-C1'	-3.34	1.48	1.53
2	D	900	ADX	C2'-C1'	-3.33	1.48	1.53
2	D	900	ADX	O2'-C2'	-3.22	1.35	1.43
2	A	900	ADX	O2'-C2'	-3.20	1.35	1.43
2	C	900	ADX	O2'-C2'	-3.19	1.35	1.43
2	E	900	ADX	C2'-C1'	-3.17	1.49	1.53
2	G	900	ADX	O2'-C2'	-3.12	1.35	1.43
2	E	900	ADX	O2'-C2'	-3.06	1.35	1.43
2	E	900	ADX	C6-N6	2.97	1.44	1.34
2	A	900	ADX	PA-O3A	2.95	1.61	1.59
2	H	900	ADX	C6-N6	2.91	1.44	1.34
2	H	900	ADX	C5'-C4'	-2.90	1.42	1.51
2	D	900	ADX	PA-O3A	2.90	1.61	1.59
2	F	900	ADX	C6-N6	2.85	1.44	1.34
2	F	900	ADX	C5'-C4'	-2.83	1.42	1.51
2	B	900	ADX	O2'-C2'	-2.80	1.36	1.43
2	A	900	ADX	C5'-C4'	-2.74	1.43	1.51
2	G	900	ADX	C6-N6	2.73	1.44	1.34
2	D	900	ADX	C6-N6	2.72	1.44	1.34
2	A	900	ADX	C6-N6	2.70	1.43	1.34
2	B	900	ADX	C5'-C4'	-2.66	1.43	1.51
2	C	900	ADX	C6-N6	2.66	1.43	1.34
2	B	900	ADX	C6-N6	2.60	1.43	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	900	ADX	C5'-C4'	-2.55	1.43	1.51
2	E	900	ADX	C5'-C4'	-2.51	1.43	1.51
2	C	900	ADX	C5'-C4'	-2.43	1.44	1.51
2	D	900	ADX	C5'-C4'	-2.37	1.44	1.51
2	H	900	ADX	C2'-C3'	-2.30	1.47	1.53
2	A	900	ADX	C2'-C3'	-2.23	1.47	1.53
2	D	900	ADX	C3'-C4'	-2.18	1.47	1.53
2	G	900	ADX	C2-N3	2.14	1.35	1.32
2	D	900	ADX	C2'-C3'	-2.12	1.47	1.53
2	F	900	ADX	C2'-C3'	-2.10	1.47	1.53
2	E	900	ADX	C2'-C3'	-2.10	1.47	1.53
2	F	900	ADX	PA-O3A	2.08	1.60	1.59
2	H	900	ADX	O3'-C3'	-2.08	1.38	1.43
2	B	900	ADX	C2'-C3'	-2.08	1.47	1.53
2	A	900	ADX	C3'-C4'	-2.04	1.47	1.53
2	F	900	ADX	O3'-C3'	-2.01	1.38	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	ADX	N3-C2-N1	-4.64	121.43	128.68
2	H	900	ADX	N3-C2-N1	-4.61	121.47	128.68
2	B	900	ADX	N3-C2-N1	-4.55	121.57	128.68
2	F	900	ADX	N3-C2-N1	-4.51	121.62	128.68
2	A	900	ADX	N3-C2-N1	-4.50	121.64	128.68
2	D	900	ADX	N3-C2-N1	-4.16	122.17	128.68
2	B	900	ADX	O3A-PA-O5'	4.09	114.94	102.98
2	E	900	ADX	N3-C2-N1	-4.01	122.41	128.68
2	G	900	ADX	N3-C2-N1	-3.93	122.54	128.68
2	G	900	ADX	O3A-PA-O5'	3.36	112.78	102.98
2	E	900	ADX	C1'-N9-C4	-2.97	121.42	126.64
2	E	900	ADX	O3A-PA-O5'	2.97	111.66	102.98
2	A	900	ADX	O3A-PA-O5'	2.84	111.29	102.98
2	D	900	ADX	C1'-N9-C4	-2.81	121.70	126.64
2	H	900	ADX	C4-C5-N7	-2.56	106.74	109.40
2	D	900	ADX	O3A-PA-O5'	2.54	110.40	102.98
2	E	900	ADX	C4-C5-N7	-2.49	106.80	109.40
2	C	900	ADX	C4-C5-N7	-2.36	106.94	109.40
2	A	900	ADX	C1'-N9-C4	-2.35	122.52	126.64
2	B	900	ADX	C1'-N9-C4	-2.32	122.56	126.64
2	H	900	ADX	C1'-N9-C4	-2.31	122.59	126.64
2	F	900	ADX	O3A-PA-O5'	2.29	109.66	102.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	ADX	C1'-N9-C4	-2.27	122.64	126.64
2	C	900	ADX	O5'-C5'-C4'	2.23	116.67	108.99
2	D	900	ADX	C4-C5-N7	-2.22	107.08	109.40
2	B	900	ADX	O5'-C5'-C4'	2.18	116.51	108.99
2	F	900	ADX	C1'-N9-C4	-2.17	122.83	126.64
2	E	900	ADX	O5'-C5'-C4'	2.14	116.37	108.99
2	B	900	ADX	C4-C5-N7	-2.14	107.17	109.40
2	A	900	ADX	C4-C5-N7	-2.13	107.18	109.40
2	D	900	ADX	O5'-C5'-C4'	2.05	116.06	108.99
2	H	900	ADX	O5'-C5'-C4'	2.01	115.90	108.99
2	C	900	ADX	O3A-PA-O5'	2.01	108.84	102.98

There are no chirality outliers.

All (13) torsion outliers are listed below:

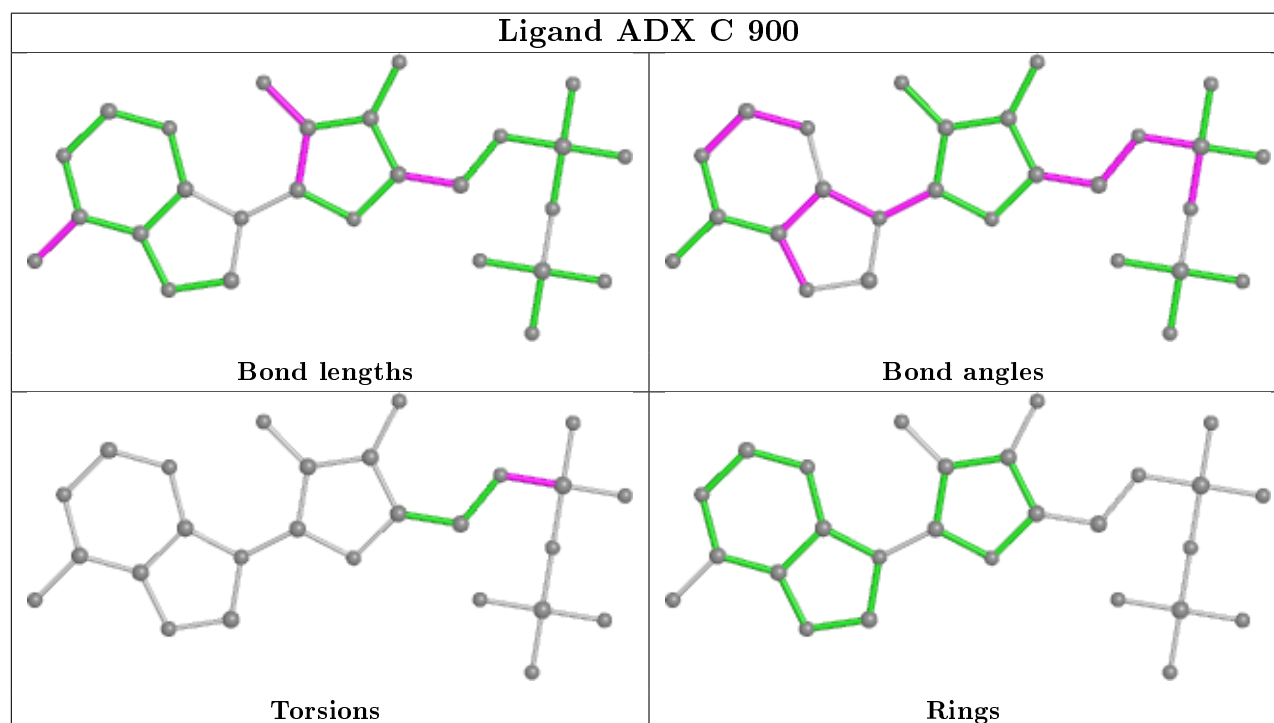
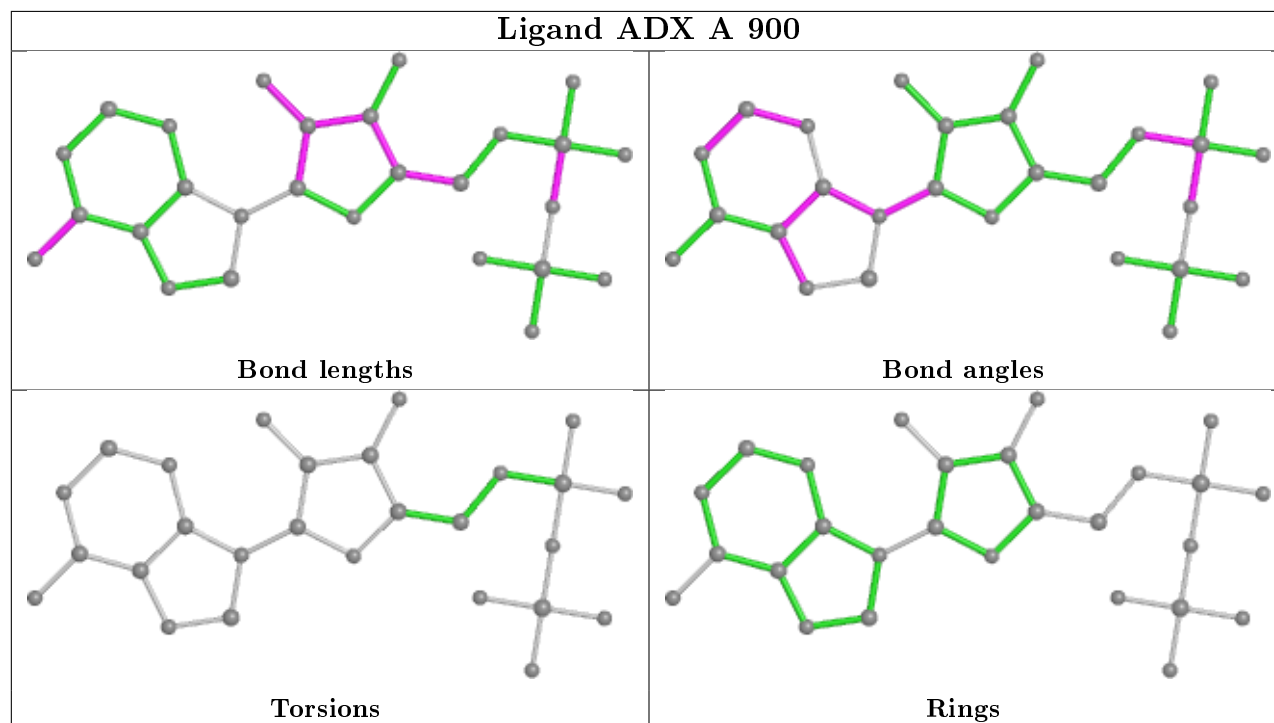
Mol	Chain	Res	Type	Atoms
2	C	900	ADX	C5'-O5'-PA-O1A
2	F	900	ADX	C5'-O5'-PA-O1A
2	F	900	ADX	C5'-O5'-PA-O3A
2	H	900	ADX	C5'-O5'-PA-O1A
2	H	900	ADX	C5'-O5'-PA-O2A
2	H	900	ADX	C5'-O5'-PA-O3A
2	C	900	ADX	C5'-O5'-PA-O2A
2	D	900	ADX	C5'-O5'-PA-O2A
2	F	900	ADX	C5'-O5'-PA-O2A
2	C	900	ADX	C5'-O5'-PA-O3A
2	E	900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

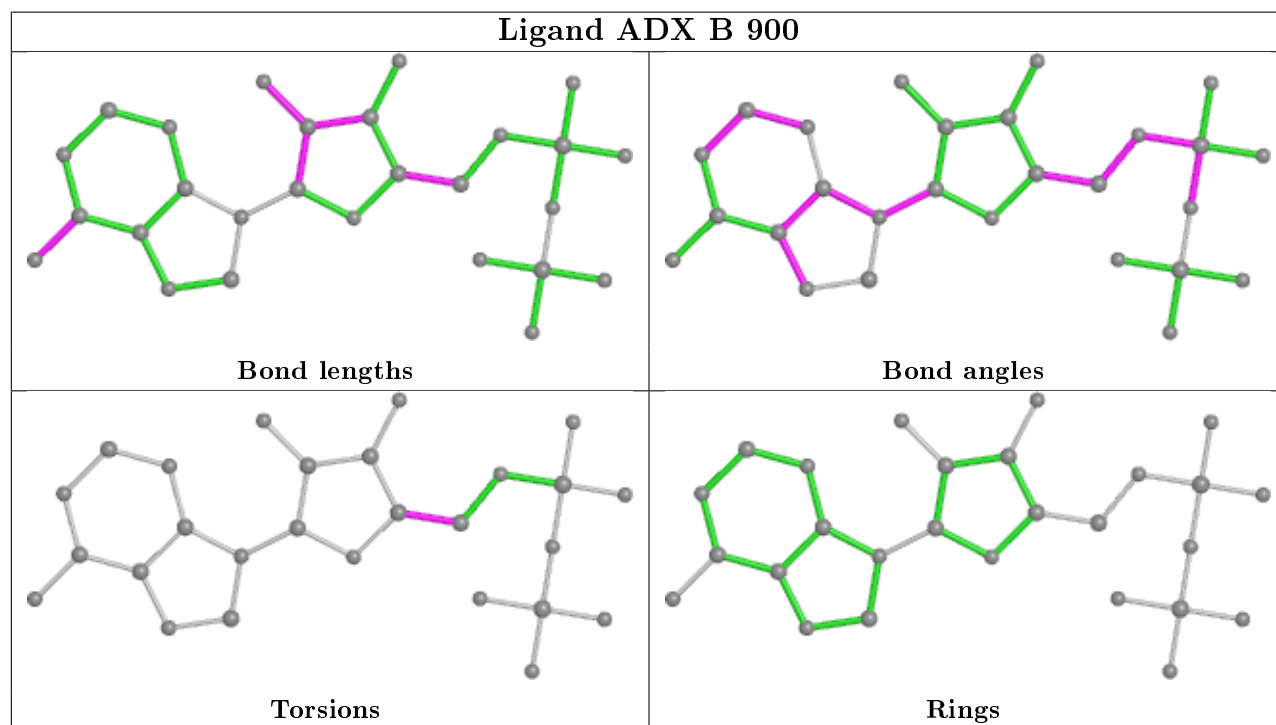
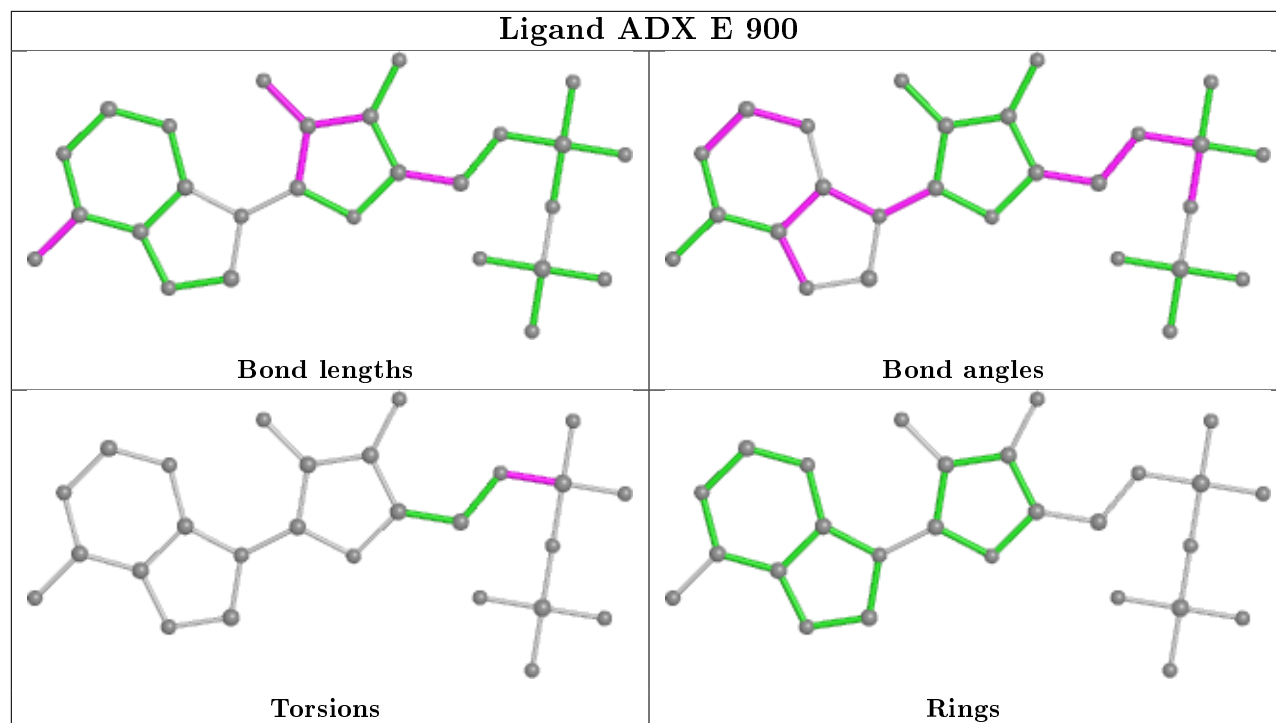
There are no ring outliers.

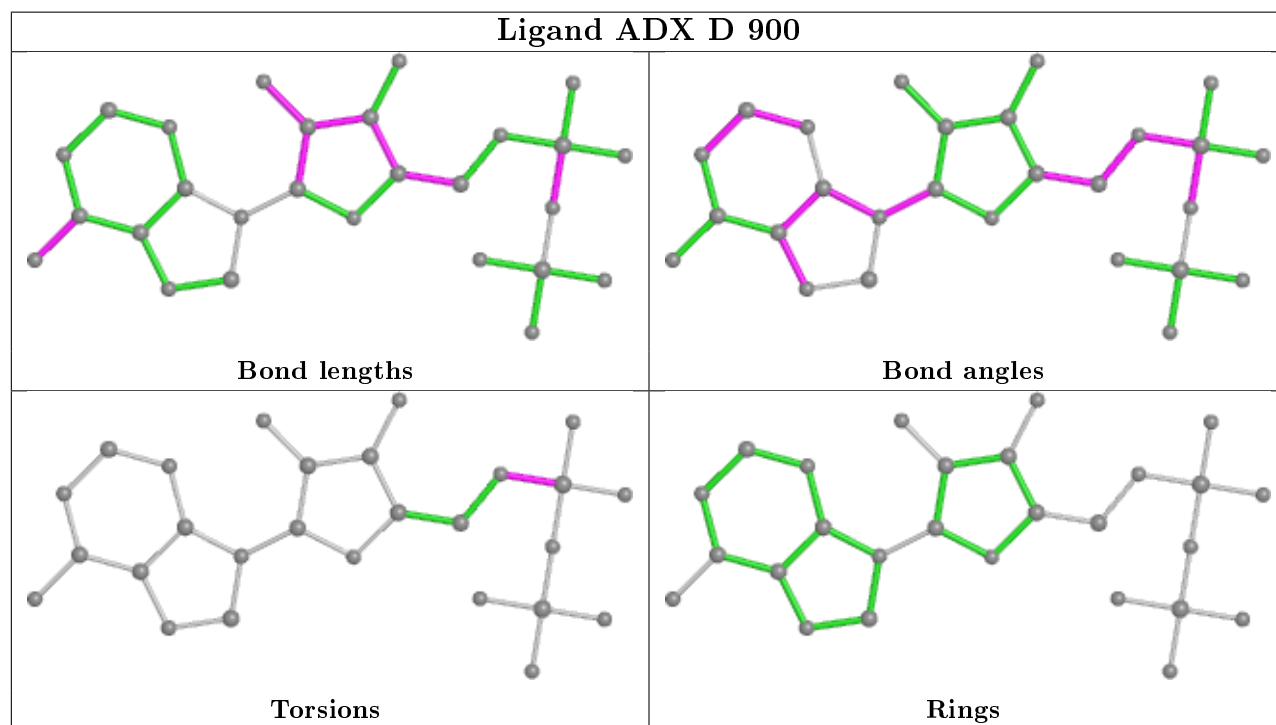
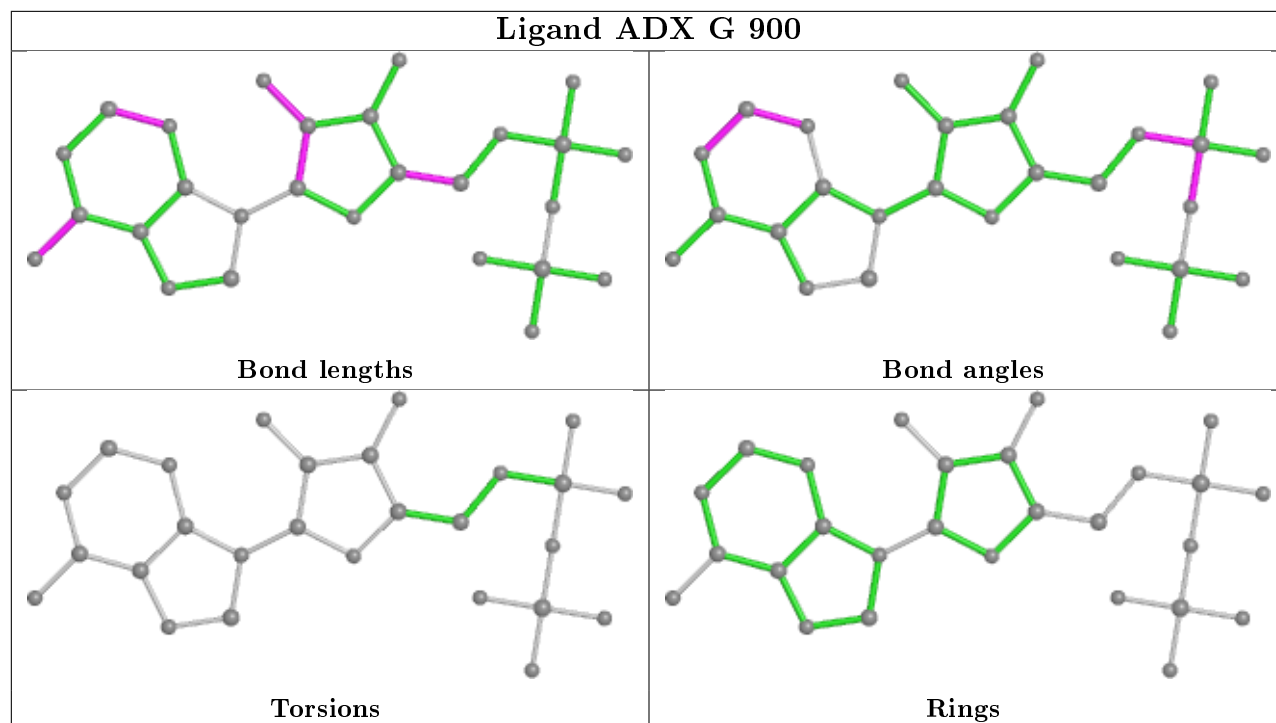
No monomer is involved in short contacts.

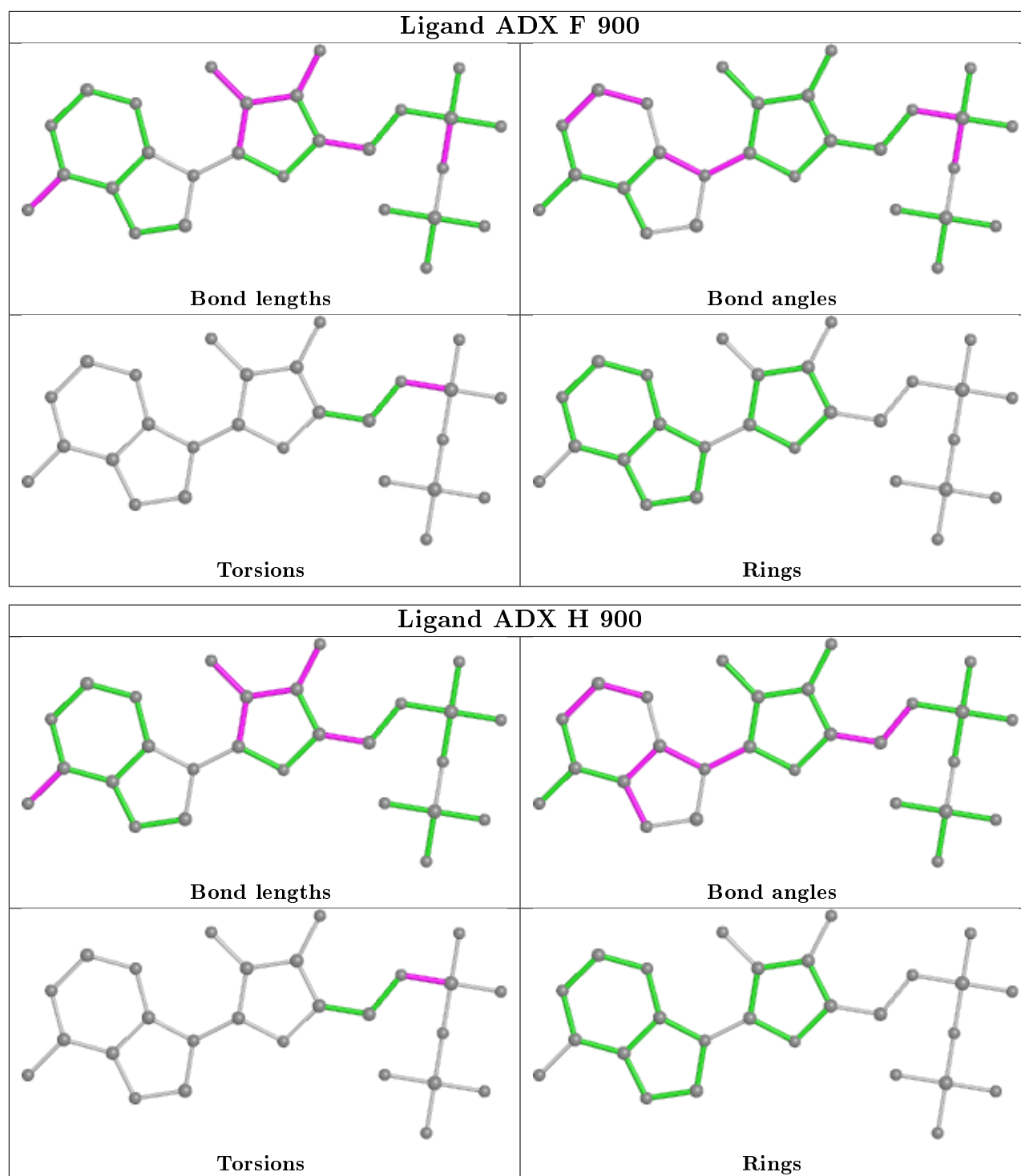
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	-0.29	3 (0%) 87 89	29, 47, 76, 106	0
1	B	404/404 (100%)	-0.33	5 (1%) 79 80	18, 39, 68, 103	0
1	C	403/404 (99%)	-0.54	1 (0%) 95 95	16, 30, 56, 70	0
1	D	401/404 (99%)	-0.23	4 (0%) 82 84	21, 43, 76, 110	0
1	E	403/404 (99%)	-0.24	3 (0%) 87 89	19, 37, 68, 99	0
1	F	401/404 (99%)	-0.06	17 (4%) 36 38	31, 53, 82, 104	0
1	G	404/404 (100%)	-0.18	4 (0%) 82 84	24, 39, 71, 108	0
1	H	381/404 (94%)	0.46	31 (8%) 12 11	47, 84, 117, 146	0
All	All	3199/3232 (98%)	-0.18	68 (2%) 63 65	16, 44, 91, 146	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	445	TYR	5.2
1	H	445	TYR	5.0
1	A	48	MET	5.0
1	H	65	PHE	4.6
1	F	425	LYS	4.5
1	H	441	LEU	4.5
1	H	411	LEU	4.4
1	H	432	PHE	4.4
1	H	63	THR	4.0
1	E	65	PHE	3.9
1	H	55	GLY	3.8
1	H	64	ASP	3.7
1	H	238	ASN	3.7
1	H	394	LYS	3.6
1	G	65	PHE	3.5
1	F	421	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	65	PHE	3.4
1	B	65	PHE	3.4
1	F	448	LEU	3.3
1	B	425	LYS	3.3
1	E	155	ASP	3.2
1	F	65	PHE	3.2
1	F	422	ALA	3.1
1	B	158	GLY	3.0
1	F	272	LYS	3.0
1	H	391	ALA	2.9
1	H	437	GLY	2.8
1	F	63	THR	2.6
1	H	302	VAL	2.6
1	H	392	TYR	2.6
1	H	433	MET	2.6
1	H	212	GLU	2.5
1	D	270	GLY	2.5
1	C	48	MET	2.5
1	D	69	LEU	2.5
1	H	431	GLY	2.5
1	F	444	TYR	2.5
1	B	154	PHE	2.4
1	F	413	ILE	2.4
1	D	65	PHE	2.4
1	H	430	ASP	2.4
1	H	271	TYR	2.4
1	F	269	MET	2.4
1	D	48	MET	2.3
1	H	155	ASP	2.3
1	H	297	LYS	2.3
1	H	61	VAL	2.3
1	H	255	HIS	2.3
1	H	235	THR	2.3
1	B	75	LEU	2.3
1	A	157	LYS	2.2
1	G	137	ILE	2.2
1	H	272	LYS	2.2
1	H	360	LYS	2.2
1	H	444	TYR	2.1
1	H	239	ALA	2.1
1	G	238	ASN	2.1
1	F	446	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	69	LEU	2.1
1	G	425	LYS	2.1
1	H	213	PRO	2.1
1	H	308	LEU	2.1
1	F	68	ASP	2.0
1	E	238	ASN	2.0
1	H	434	CYS	2.0
1	F	67	ARG	2.0
1	F	270	GLY	2.0
1	F	415	GLY	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 monosaccharides in this entry.

6.4 Ligands [i](#)

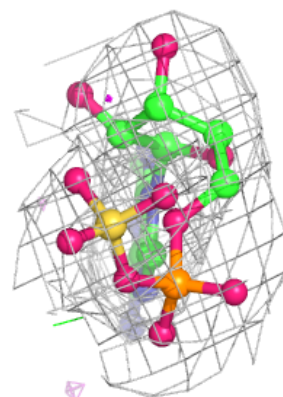
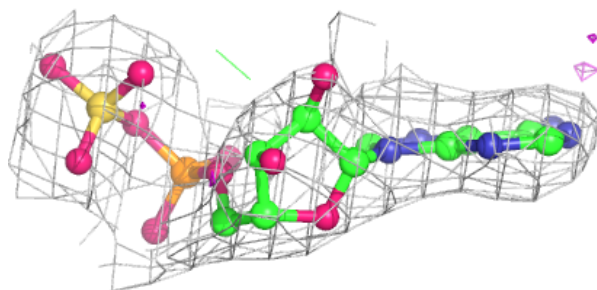
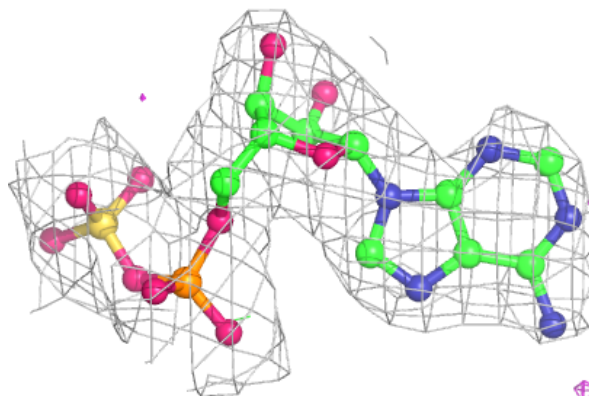
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADX	H	900	27/27	0.96	0.14	71,78,84,91	0
2	ADX	G	900	27/27	0.98	0.12	20,27,33,35	0
2	ADX	F	900	27/27	0.98	0.13	39,48,53,56	0
2	ADX	E	900	27/27	0.98	0.13	21,29,34,37	0
2	ADX	C	900	27/27	0.99	0.12	17,23,30,32	0
2	ADX	D	900	27/27	0.99	0.13	21,28,30,32	0
2	ADX	A	900	27/27	0.99	0.10	27,32,36,38	0
2	ADX	B	900	27/27	0.99	0.13	22,29,34,38	0

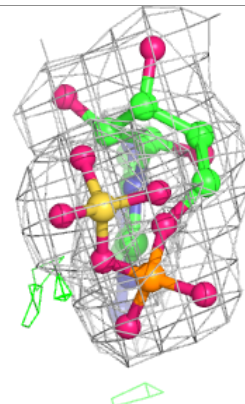
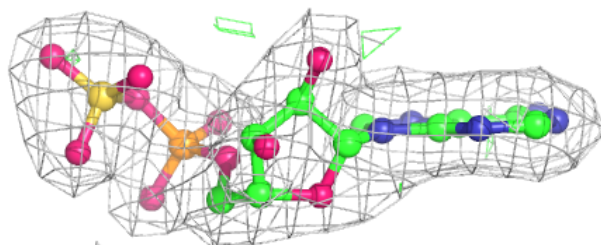
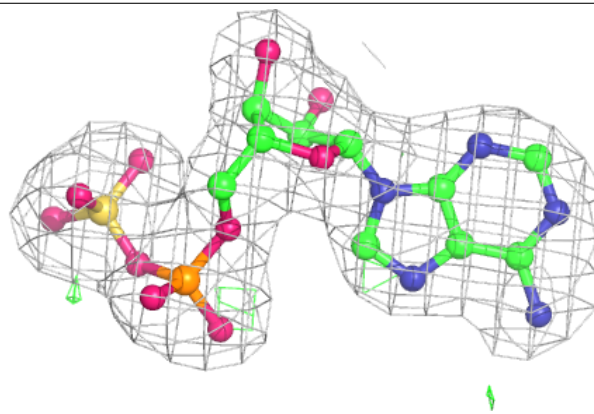
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

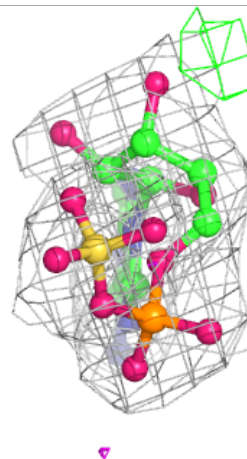
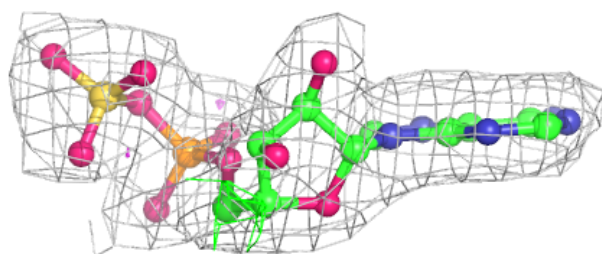
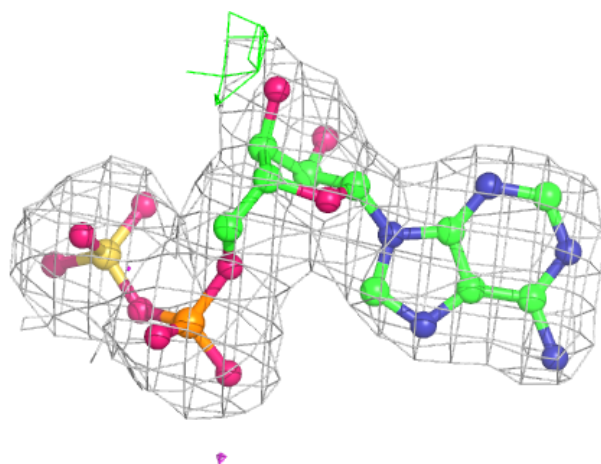
**Electron density around ADX G 900:**

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



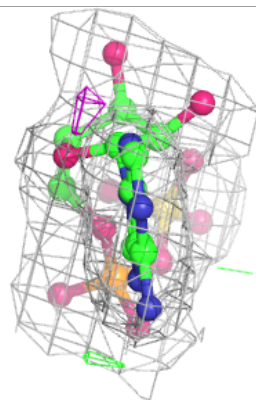
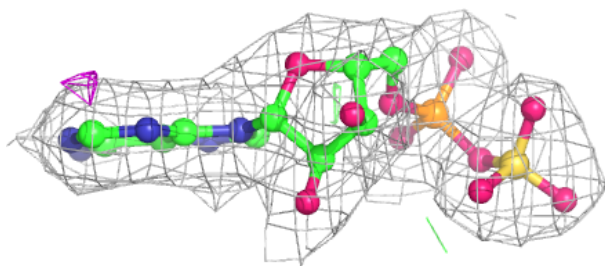
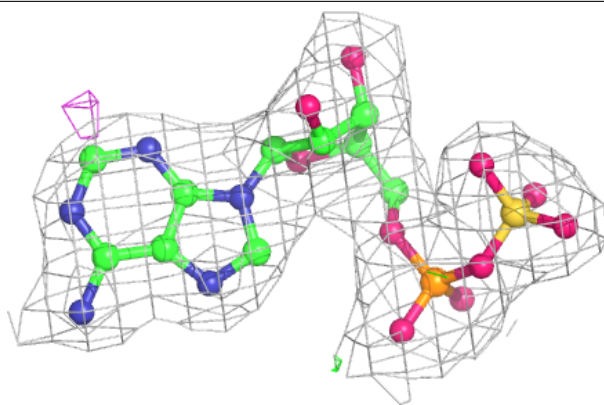
Electron density around ADX F 900:

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

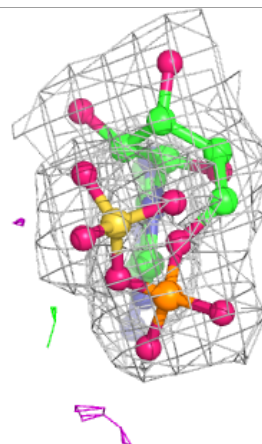
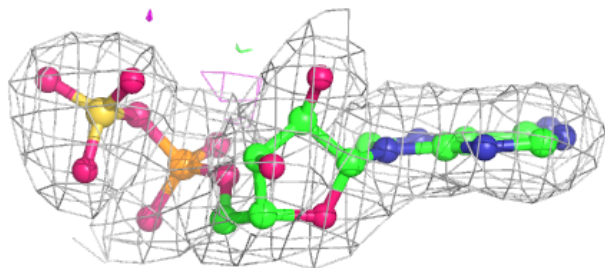
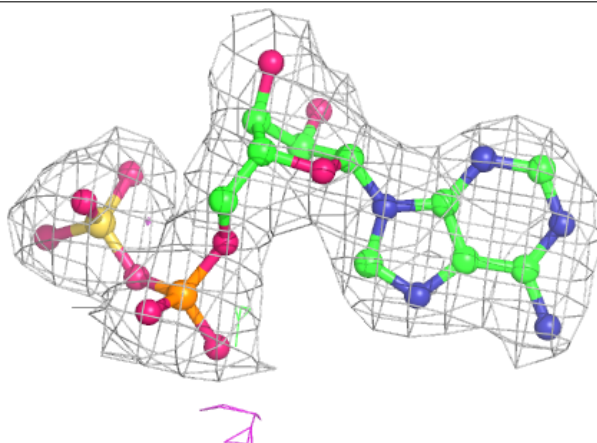


Electron density around ADX E 900:

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

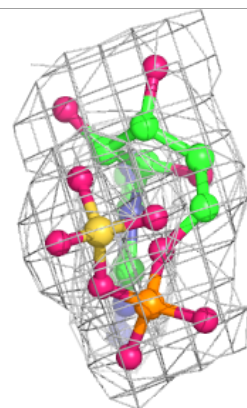
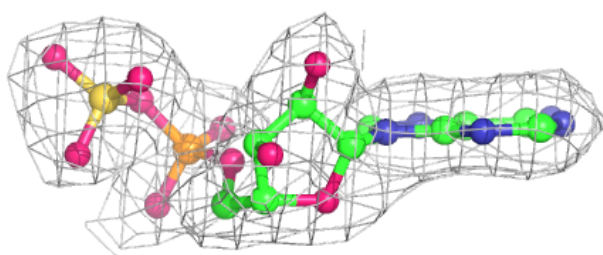
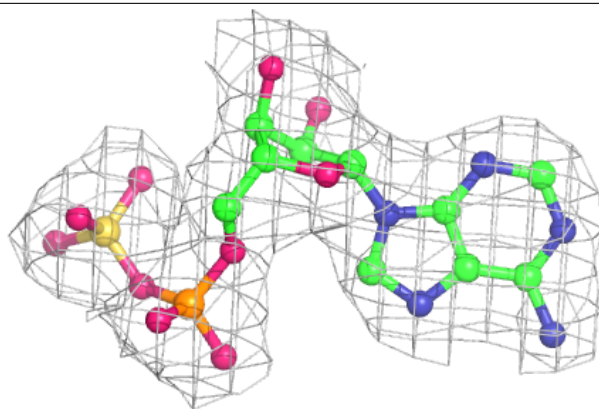
**Electron density around ADX C 900:**

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

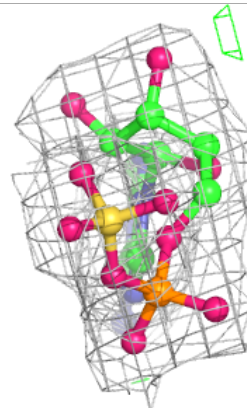
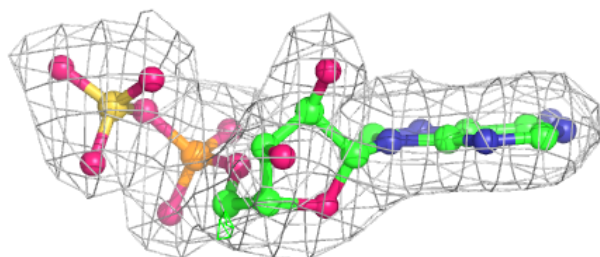
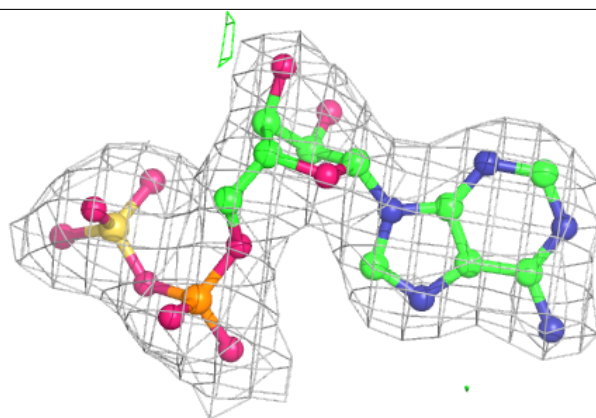


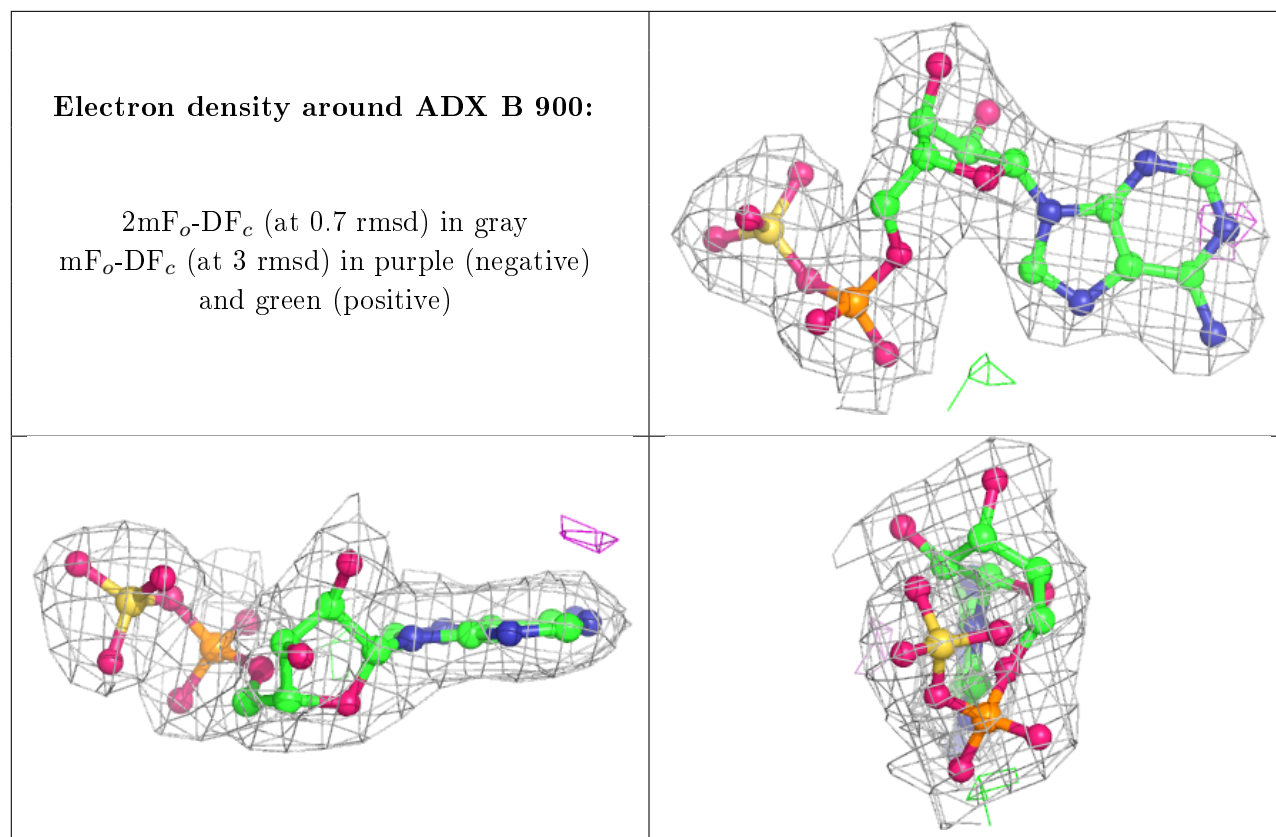
Electron density around ADX D 900:

$2mF_o-DF_c$ (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.