Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2024 – 01:17 PM EST

PDB ID	:	2FJA
Title	:	adenosine 5'-phosphosulfate reductase in complex with substrate
Authors	:	Schiffer, A.; Fritz, G.; Kroneck, P.M.; Ermler, U.
Deposited on	:	2006-01-02
Resolution	:	2.00 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 (i) 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 (1)) were used in the production of this report:

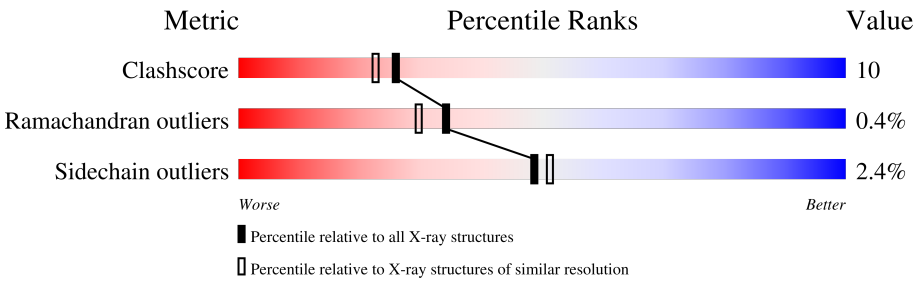
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	643	80% 18% •
1	C	643	80% 19% •
2	B	150	73% 24% • •
2	D	150	76% 21% •••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SF4	D	3110	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14060 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.

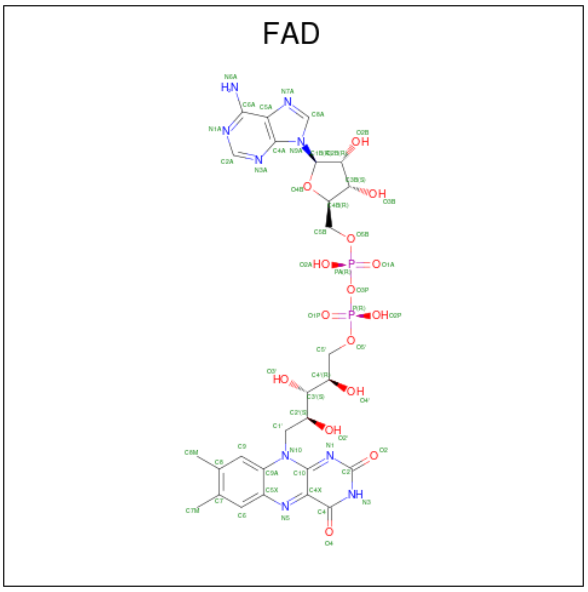
- Molecule 1 is a protein called adenylylsulfate reductase, subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	642	5191	3359	855	948	29	0	6	0
1	C	642	5191	3358	854	950	29	0	6	0

- Molecule 2 is a protein called adenylylsulfate reductase, subunit B.

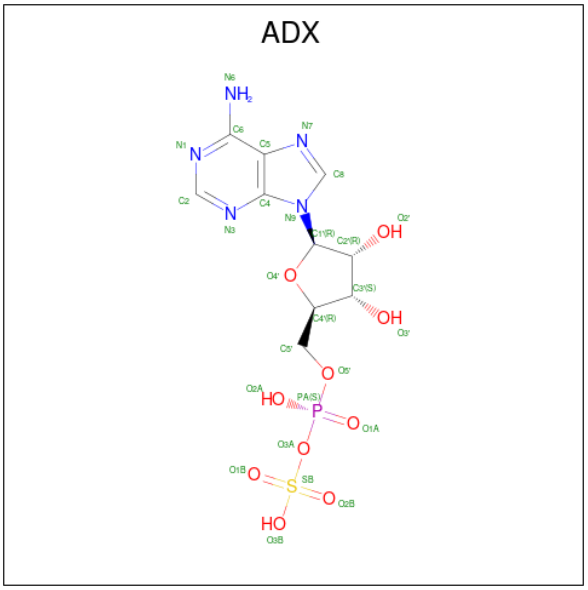
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	149	1179	751	193	219	16	11	2	0
2	D	149	1174	745	193	220	16	9	1	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



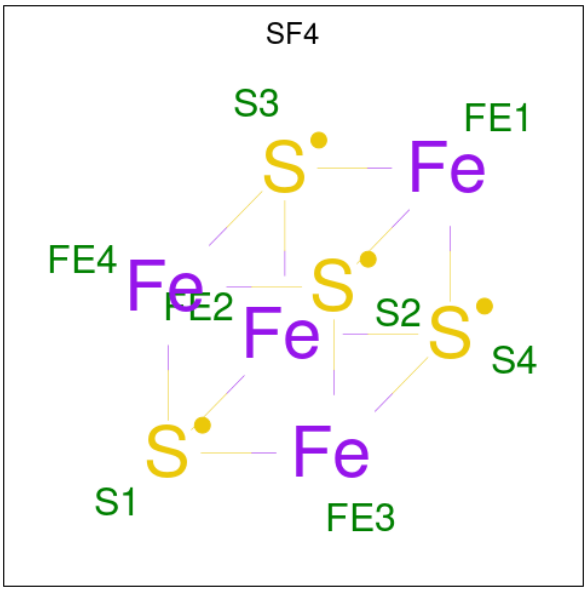
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
3	C	1	53	27	9	15	2	0	0

- Molecule 4 is ADENOSINE-5'-PHOSPHOSULFATE (three-letter code: ADX) (formula: $C_{10}H_{14}N_5O_{10}PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	C	1	54	20	10	20	2	2	0	1
			Total	C	N	O	P	S		
4	C	1	54	20	10	20	2	2	0	1

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	B	1	8	4	4	0	0
			Total	Fe	S		
5	B	1	8	4	4	2	0
			Total	Fe	S		
5	D	1	8	4	4	0	0
			Total	Fe	S		
5	D	1	8	4	4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	413	413	413	0	0
			Total	O		
6	C	445	445	445	0	0
			Total	O		
6	B	102	102	102	0	0
			Total	O		
6	D	119	119	119	0	0

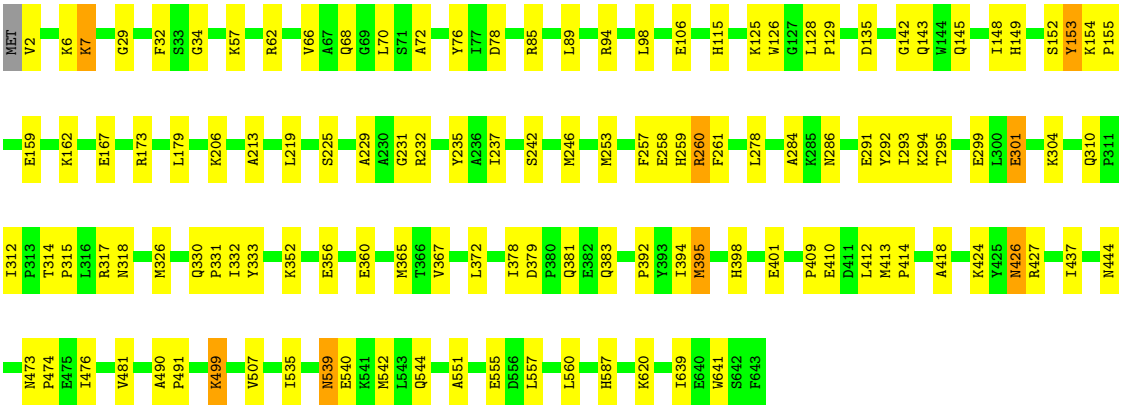
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

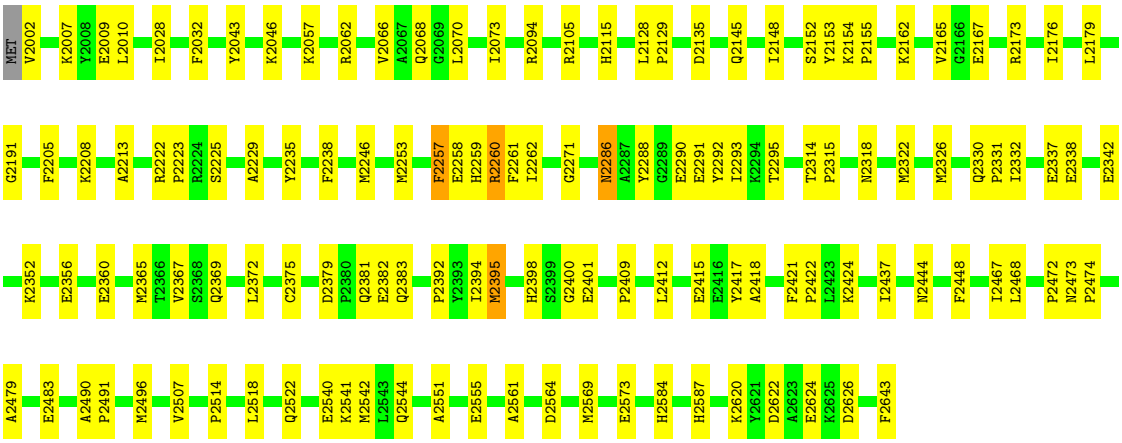
• Molecule 1: adenylylsulfate reductase, subunit A

Chain A: 80% 18% •



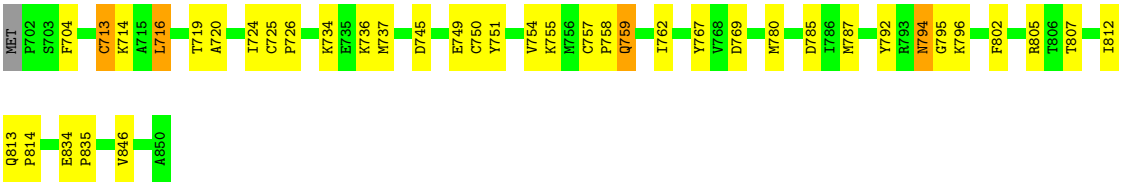
• Molecule 1: adenylylsulfate reductase, subunit A

Chain C: 80% 19% •



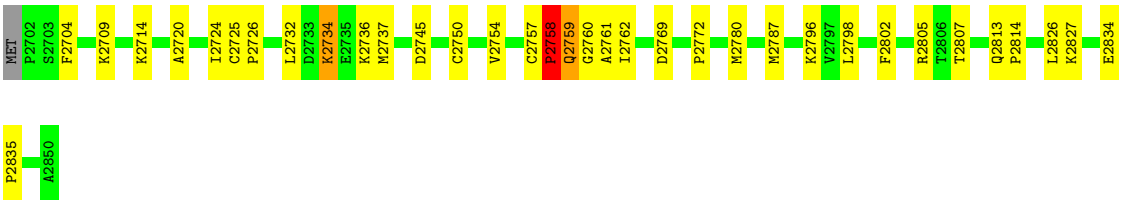
• Molecule 2: adenylylsulfate reductase, subunit B

Chain B: 73% 24% • •



• Molecule 2: adenylylsulfate reductase, subunit B

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.60Å 113.50Å 193.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	89.9 (30.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.174 , 0.208	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14060	wwPDB-VP
Average B, all atoms ($Å^2$)	23.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADX, SF4, FAD

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	0.31	0/5356	0.58	0/7248
1	C	0.32	0/5356	0.59	0/7249
2	B	0.30	0/1217	0.62	0/1643
2	D	0.30	0/1208	0.63	0/1631
All	All	0.31	0/13137	0.59	0/17771

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5191	0	5089	108	0
1	C	5191	0	5082	99	0
2	B	1179	0	1160	44	0
2	D	1174	0	1148	35	0
3	A	53	0	29	2	0
3	C	53	0	29	4	0
4	C	108	0	48	15	0
5	B	16	0	0	1	0
5	D	16	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	413	0	0	6	0
6	B	102	0	0	3	0
6	C	445	0	0	2	0
6	D	119	0	0	2	0
All	All	14060	0	12585	268	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 10.

All (268) 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)
4:C:1200[B]:ADX:O2A	4:C:1200[B]:ADX:H8	1.21	1.32
4:C:3200[B]:ADX:O2A	4:C:3200[B]:ADX:H8	1.29	1.28
4:C:1200[B]:ADX:O2A	4:C:1200[B]:ADX:C8	1.95	1.12
4:C:3200[B]:ADX:O2A	4:C:3200[B]:ADX:C8	2.01	1.09
2:B:713:CYS:HB3	2:B:716:LEU:HD21	1.43	0.98
1:C:2379:ASP:H	1:C:2383:GLN:NE2	1.64	0.94
1:C:2379:ASP:H	1:C:2383:GLN:HE21	0.97	0.94
2:D:2757[B]:CYS:SG	2:D:2761:ALA:HB3	2.15	0.87
2:B:734:LYS:HD2	2:B:734:LYS:H	1.44	0.82
1:A:378:ILE:HG12	1:A:383:GLN:HE21	1.45	0.81
1:C:2379:ASP:N	1:C:2383:GLN:HE21	1.79	0.80
4:C:1200[B]:ADX:H8	4:C:1200[B]:ADX:PA	2.22	0.79
1:A:259:HIS:HD2	1:A:401:GLU:H	1.29	0.78
4:C:3200[B]:ADX:H8	4:C:3200[B]:ADX:PA	2.23	0.78
1:C:2330:GLN:HG2	1:C:2332:ILE:HD13	1.66	0.77
1:C:2259:HIS:HD2	1:C:2401:GLU:H	1.32	0.76
1:C:2225:SER:HB3	1:C:2229:ALA:HB3	1.70	0.73
1:A:106:GLU:HB3	1:A:639:ILE:HD13	1.71	0.73
1:A:352:LYS:O	1:A:356:GLU:HG3	1.89	0.72
1:A:225:SER:HB3	1:A:229:ALA:HB3	1.70	0.72
1:A:145:GLN:NE2	4:C:1200[B]:ADX:O3'	2.23	0.72
1:A:540:GLU:O	1:A:544:GLN:HG3	1.92	0.70
1:C:2352:LYS:O	1:C:2356:GLU:HG3	1.91	0.70
1:A:426:ASN:HD21	1:A:427:ARG:HH11	1.39	0.70
1:C:2541:LYS:HA	1:C:2541:LYS:HE2	1.73	0.70
1:A:6:LYS:HB3	1:A:7:LYS:HD3	1.74	0.69
2:B:713:CYS:CB	2:B:716:LEU:HD21	2.21	0.68
1:A:115:HIS:HD2	2:B:834:GLU:OE2	1.77	0.68
1:A:539:ASN:C	1:A:539:ASN:HD22	1.96	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2418:ALA:HB1	1:C:2424:LYS:HE3	1.76	0.68
1:C:2145:GLN:NE2	4:C:3200[B]:ADX:O3'	2.22	0.67
2:D:2709:LYS:HB2	2:D:2761:ALA:HA	1.76	0.67
1:C:2261:PHE:CZ	4:C:3200[B]:ADX:O3B	2.48	0.67
1:A:378:ILE:HG12	1:A:383:GLN:NE2	2.10	0.66
6:A:6226:HOH:O	1:C:2542[B]:MET:HE1	1.93	0.66
2:B:794:ASN:ND2	2:B:796:LYS:H	1.93	0.66
2:D:2796:LYS:HE2	2:D:2798:LEU:HD21	1.77	0.66
1:C:2286:ASN:HD22	1:C:2286:ASN:C	1.99	0.65
1:A:66:VAL:HG12	1:A:66:VAL:O	1.97	0.65
2:B:794:ASN:C	2:B:794:ASN:HD22	2.00	0.65
1:A:162:LYS:HE3	1:A:167:GLU:HB2	1.79	0.65
1:A:179:LEU:HG	1:A:246:MET:HB2	1.78	0.65
1:A:94:ARG:HG3	1:A:641:TRP:CE3	2.31	0.64
2:D:2780:MET:HB2	2:D:2787:MET:HB2	1.80	0.64
2:D:2757[B]:CYS:SG	2:D:2758:PRO:HD2	2.38	0.63
1:C:2066:VAL:HG13	1:C:2070:LEU:HG	1.79	0.62
1:C:2398:HIS:NE2	4:C:3200[A]:ADX:O1B	2.31	0.62
2:D:2720:ALA:HB3	5:D:3110:SF4:S1	2.39	0.62
1:C:2286:ASN:ND2	1:C:2288:TYR:H	1.98	0.62
1:C:2261:PHE:HZ	4:C:3200[B]:ADX:O3B	1.83	0.61
1:A:235:TYR:HA	3:A:1000:FAD:HM83	1.82	0.61
1:A:379:ASP:OD2	1:A:381:GLN:HG2	2.00	0.61
1:A:551:ALA:O	1:A:555:GLU:HG3	2.01	0.61
1:C:2259:HIS:CD2	1:C:2401:GLU:H	2.17	0.61
1:C:2115:HIS:HD2	2:D:2834:GLU:OE2	1.84	0.61
1:C:2379:ASP:OD2	1:C:2381:GLN:HG2	2.01	0.60
1:A:261:PHE:HZ	4:C:1200[B]:ADX:O3B	1.83	0.60
1:C:2551:ALA:O	1:C:2555:GLU:HG3	2.01	0.60
2:D:2759:GLN:N	2:D:2759:GLN:CD	2.55	0.60
1:C:2293:ILE:HG23	6:C:5365:HOH:O	2.01	0.60
2:D:2734:LYS:H	2:D:2734:LYS:HD2	1.66	0.59
1:A:499:LYS:HB2	1:A:499:LYS:NZ	2.18	0.59
1:A:259:HIS:CD2	1:A:401:GLU:H	2.17	0.59
1:A:365[B]:MET:HE3	3:A:1000:FAD:H6	1.85	0.58
1:A:68:GLN:HG2	2:B:750:CYS:HB2	1.85	0.58
1:C:2179:LEU:HG	1:C:2246[B]:MET:HB2	1.85	0.58
1:A:418:ALA:O	1:A:424:LYS:HE3	2.03	0.57
1:C:2365[B]:MET:HE3	3:C:3000:FAD:H6	1.86	0.57
1:A:115:HIS:HE1	6:A:5205:HOH:O	1.88	0.57
1:C:2028[B]:ILE:HD12	1:C:2176:ILE:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2066:VAL:O	1:C:2066:VAL:HG12	2.05	0.57
2:B:757:CYS:O	2:B:759:GLN:N	2.36	0.57
1:A:253:MET:HG2	1:A:620:LYS:HB2	1.87	0.56
1:C:2068:GLN:HG2	2:D:2750:CYS:HB2	1.86	0.56
1:C:2540:GLU:O	1:C:2544:GLN:HG3	2.05	0.56
2:D:2759:GLN:CD	2:D:2759:GLN:H	2.09	0.56
1:C:2330:GLN:HG2	1:C:2332:ILE:CD1	2.34	0.56
2:D:2827:LYS:HE3	6:D:6005:HOH:O	2.04	0.56
1:C:2115:HIS:HE1	6:D:5004:HOH:O	1.88	0.56
1:A:154:LYS:HB3	1:A:155:PRO:HD3	1.86	0.56
1:C:2068:GLN:HE22	1:C:2367:VAL:H	1.55	0.55
6:A:5720:HOH:O	2:B:796:LYS:HE3	2.06	0.55
2:D:2758:PRO:O	2:D:2760:GLY:N	2.40	0.55
1:A:301:GLU:HG2	1:A:304:LYS:HZ3	1.72	0.54
1:A:70:LEU:HA	1:A:365[B]:MET:HB3	1.88	0.54
1:C:2292:TYR:HA	1:C:2295:THR:OG1	2.08	0.54
2:B:749:GLU:HG3	2:B:767:TYR:CZ	2.42	0.54
1:A:149:HIS:HD2	1:A:360:GLU:OE2	1.91	0.54
1:A:312:ILE:O	1:A:317[B]:ARG:NH1	2.40	0.54
1:C:2043:TYR:O	1:C:2046:LYS:HE2	2.08	0.54
1:C:2179:LEU:HG	1:C:2246[A]:MET:HB3	1.90	0.54
1:C:2235:TYR:HA	3:C:3000:FAD:HM83	1.90	0.53
1:A:398:HIS:NE2	4:C:1200[A]:ADX:O1B	2.41	0.53
1:A:57:LYS:O	1:A:173:ARG:HA	2.08	0.53
1:A:261:PHE:CZ	4:C:1200[B]:ADX:O3B	2.61	0.53
1:A:383:GLN:NE2	6:A:5508:HOH:O	2.41	0.53
1:A:639:ILE:N	1:A:639:ILE:HD12	2.24	0.53
1:A:68:GLN:HE22	1:A:367:VAL:H	1.57	0.52
1:A:291:GLU:HG2	1:A:293:ILE:HG13	1.91	0.52
1:C:2135:ASP:HB2	6:C:5889:HOH:O	2.09	0.52
2:B:780:MET:SD	2:B:787[A]:MET:HE3	2.49	0.52
1:C:2154:LYS:HB3	1:C:2155:PRO:HD3	1.91	0.52
1:C:2259:HIS:HD2	1:C:2401:GLU:N	2.06	0.52
1:C:2176:ILE:HG22	1:C:2246[A]:MET:SD	2.49	0.52
1:C:2479:ALA:O	1:C:2483:GLU:HG3	2.09	0.51
1:A:260:ARG:HG3	1:A:392:PRO:HB3	1.93	0.51
1:C:2094[A]:ARG:NH1	1:C:2643:PHE:HA	2.26	0.51
1:A:89:LEU:HD13	2:B:846:VAL:HG22	1.93	0.51
1:A:286:ASN:HA	1:A:332[B]:ILE:HD13	1.92	0.51
1:C:2057:LYS:O	1:C:2173:ARG:HA	2.11	0.51
1:C:2467:ILE:HA	1:C:2472:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:780:MET:HB2	2:B:787[B]:MET:HB2	1.92	0.51
1:C:2253:MET:HG2	1:C:2620:LYS:HB2	1.93	0.50
1:A:409:PRO:HG2	1:A:412:LEU:HB2	1.93	0.50
1:C:2257:PHE:O	1:C:2584:HIS:HD2	1.94	0.50
1:A:259:HIS:CD2	1:A:401:GLU:HG2	2.47	0.50
1:C:2070:LEU:HA	1:C:2365[A]:MET:HB2	1.92	0.50
1:C:2010:LEU:HD13	1:C:2496:MET:HG2	1.94	0.50
1:A:6:LYS:HB3	1:A:7:LYS:CD	2.41	0.50
1:A:159:GLU:OE1	2:B:812[B]:ILE:HG12	2.12	0.50
1:A:94:ARG:NH1	1:A:98:LEU:HD11	2.26	0.49
1:A:383:GLN:HG2	6:A:5805:HOH:O	2.11	0.49
2:B:713:CYS:SG	2:B:719:THR:HA	2.52	0.49
1:A:314:THR:N	1:A:315:PRO:HD2	2.27	0.49
1:C:2473:ASN:N	1:C:2474:PRO:HD3	2.28	0.49
1:A:301:GLU:O	1:A:304:LYS:HG3	2.13	0.49
1:C:2002:VAL:N	2:D:2745:ASP:OD1	2.46	0.49
1:A:259:HIS:HD2	1:A:401:GLU:N	2.05	0.49
1:A:418:ALA:HB1	1:A:424:LYS:CE	2.43	0.49
1:C:2286:ASN:ND2	1:C:2290:GLU:H	2.11	0.49
1:C:2338:GLU:O	1:C:2342:GLU:HG3	2.14	0.48
1:A:372:LEU:C	1:A:372:LEU:HD23	2.34	0.48
1:C:2258:GLU:HB3	1:C:2587:HIS:HB3	1.96	0.48
1:C:2360:GLU:HB2	2:D:2802:PHE:CE2	2.49	0.48
1:C:2365[B]:MET:CE	3:C:3000:FAD:H6	2.43	0.48
2:B:794:ASN:HD22	2:B:796:LYS:H	1.58	0.48
1:A:89:LEU:CD1	2:B:846:VAL:HG22	2.44	0.48
1:A:125:LYS:HD2	6:B:5731:HOH:O	2.14	0.48
1:A:206:LYS:HE2	1:A:476:ILE:CD1	2.44	0.48
2:B:780:MET:HB2	2:B:787[A]:MET:HB3	1.94	0.48
2:B:794:ASN:HD22	2:B:795:GLY:N	2.12	0.48
2:D:2709:LYS:HG3	2:D:2760:GLY:O	2.13	0.47
1:A:360:GLU:HB2	2:B:802:PHE:CE2	2.49	0.47
1:C:2490:ALA:HB3	1:C:2491:PRO:HD3	1.96	0.47
1:C:2286:ASN:C	1:C:2286:ASN:ND2	2.66	0.47
1:C:2569:MET:O	1:C:2573:GLU:HG3	2.15	0.47
1:A:293:ILE:C	1:A:293:ILE:HD12	2.35	0.47
1:A:473:ASN:N	1:A:474:PRO:HD3	2.29	0.47
1:C:2394:ILE:C	1:C:2395:MET:HG3	2.34	0.47
1:C:2260:ARG:HH21	1:C:2584:HIS:HE1	1.62	0.47
1:C:2259:HIS:CD2	1:C:2400:GLY:HA2	2.49	0.47
2:B:794:ASN:HD21	2:B:796:LYS:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ALA:HB1	1:A:424:LYS:HE3	1.97	0.46
1:A:394:ILE:C	1:A:395:MET:HG3	2.34	0.46
1:C:2271:GLY:H	1:C:2369:GLN:HE21	1.62	0.46
1:A:258:GLU:HB3	1:A:587:HIS:HB3	1.96	0.46
2:B:751:TYR:O	2:B:755:LYS:HG3	2.16	0.46
2:D:2834:GLU:HB3	2:D:2835:PRO:HA	1.97	0.46
1:C:2381:GLN:HG3	1:C:2382:GLU:HG2	1.96	0.46
2:D:2736:LYS:O	2:D:2737:MET:HB2	2.15	0.46
1:A:7:LYS:HD3	1:A:7:LYS:N	2.30	0.46
1:A:312:ILE:N	1:A:312:ILE:HD12	2.30	0.46
1:A:126:TRP:O	2:B:812[B]:ILE:HD11	2.16	0.46
1:A:410:GLU:HG2	6:A:5806:HOH:O	2.16	0.46
1:A:542[B]:MET:SD	1:C:2331:PRO:HG3	2.55	0.46
1:A:476:ILE:HD12	1:A:481:VAL:HG21	1.98	0.46
1:C:2622:ASP:O	1:C:2626:ASP:N	2.49	0.45
1:C:2322:MET:HB3	1:C:2326:MET:HE2	1.99	0.45
1:A:292:TYR:HA	1:A:295:THR:OG1	2.17	0.45
1:A:426:ASN:ND2	1:A:427:ARG:HH11	2.11	0.45
1:C:2372:LEU:C	1:C:2372:LEU:HD23	2.37	0.45
1:A:6:LYS:HB3	1:A:7:LYS:CE	2.47	0.45
1:A:413:MET:HA	1:A:414:PRO:HD3	1.82	0.45
1:C:2062:ARG:CG	2:D:2724:ILE:HD11	2.47	0.45
1:A:142:GLY:HA3	1:A:278:LEU:HD13	1.99	0.45
1:C:2337:GLU:HG2	1:C:2338:GLU:N	2.31	0.45
2:B:725:CYS:HA	2:B:726:PRO:HD3	1.83	0.45
1:A:66:VAL:HG13	1:A:70:LEU:HG	1.98	0.45
1:C:2260:ARG:HG3	1:C:2392:PRO:HB3	1.99	0.45
1:C:2191:GLY:HA3	1:C:2205:PHE:O	2.17	0.44
2:B:757:CYS:SG	2:B:762:ILE:HD12	2.58	0.44
1:A:232:ARG:HD2	2:B:767:TYR:CE1	2.52	0.44
2:B:780:MET:HG3	6:B:5713:HOH:O	2.17	0.44
2:D:2732:LEU:HD21	5:D:3110:SF4:S4	2.58	0.44
1:A:310:GLN:HA	1:A:310:GLN:NE2	2.33	0.44
1:A:326[A]:MET:SD	1:A:535:ILE:CD1	3.06	0.44
2:B:754:VAL:HG22	2:B:762:ILE:HG22	2.00	0.44
2:B:794:ASN:ND2	2:B:794:ASN:C	2.68	0.44
1:C:2260:ARG:HH21	1:C:2584:HIS:CE1	2.35	0.44
1:A:539:ASN:ND2	1:A:539:ASN:C	2.68	0.44
1:C:2208:LYS:HB3	1:C:2472:PRO:HG2	1.98	0.44
1:A:326[A]:MET:SD	1:A:535:ILE:HD12	2.58	0.43
1:C:2330:GLN:HB3	1:C:2331:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2518:LEU:O	1:C:2522:GLN:HG3	2.18	0.43
2:B:792:TYR:HB2	2:B:796:LYS:HB3	2.00	0.43
1:C:2514:PRO:HD3	1:C:2561:ALA:O	2.19	0.43
2:D:2757[B]:CYS:SG	2:D:2758:PRO:CD	3.04	0.43
1:C:2238:PHE:CZ	2:D:2726:PRO:HB2	2.53	0.43
4:C:3200[A]:ADX:O1B	4:C:3200[A]:ADX:H5'	2.19	0.43
1:A:68:GLN:HG2	2:B:750:CYS:CB	2.47	0.43
2:B:736:LYS:O	2:B:737:MET:HB2	2.19	0.43
2:D:2757[A]:CYS:SG	2:D:2762:ILE:HD12	2.59	0.43
1:C:2152:SER:C	1:C:2155:PRO:HD2	2.39	0.43
1:A:152:SER:C	1:A:155:PRO:HD2	2.40	0.43
1:A:242:SER:O	1:A:246:MET:HG2	2.19	0.42
1:A:507:VAL:CG1	2:D:2704:PHE:HB3	2.50	0.42
1:C:2009:GLU:HB3	1:C:2564:ASP:HA	1.99	0.42
1:C:2418:ALA:HB1	1:C:2424:LYS:CE	2.46	0.42
1:A:213:ALA:HB2	1:A:437:ILE:HD11	2.00	0.42
1:C:2375:CYS:HB3	2:D:2772:PRO:HD2	2.01	0.42
2:B:805:ARG:HG2	2:B:807:THR:H	1.84	0.42
1:A:115:HIS:HD2	2:B:834:GLU:CD	2.23	0.42
1:C:2073:ILE:HG13	1:C:2148:ILE:HD13	2.01	0.42
1:C:2259:HIS:CD2	1:C:2401:GLU:HG2	2.55	0.42
1:C:2162:LYS:HE2	1:C:2167:GLU:HB3	2.02	0.42
1:A:293:ILE:HD12	1:A:294:LYS:N	2.35	0.42
1:C:2213:ALA:HB2	1:C:2437:ILE:HD11	2.02	0.42
1:C:2409:PRO:HG2	1:C:2412:LEU:HB2	2.02	0.42
1:C:2467:ILE:HA	1:C:2472:PRO:CD	2.48	0.42
1:A:68:GLN:NE2	1:A:367:VAL:H	2.17	0.41
1:A:94:ARG:NH1	1:A:98:LEU:CD1	2.83	0.41
1:C:2468:LEU:HD12	2:D:2826:LEU:CD2	2.50	0.41
2:D:2805:ARG:HG2	2:D:2807:THR:H	1.85	0.41
1:A:2:VAL:N	2:B:745:ASP:OD1	2.53	0.41
1:C:2128:LEU:HA	1:C:2129:PRO:HD3	1.94	0.41
1:C:2238:PHE:CE2	2:D:2726:PRO:HB2	2.54	0.41
1:A:557:LEU:HD22	1:A:560:LEU:HD11	2.02	0.41
2:D:2714:LYS:HE3	2:D:2737:MET:HE2	2.03	0.41
2:D:2762:ILE:HD11	5:D:3110:SF4:S2	2.59	0.41
1:A:70:LEU:HD12	1:A:153:TYR:CE2	2.56	0.41
1:A:76:TYR:CE2	1:A:78:ASP:HB2	2.56	0.41
1:A:85:ARG:CZ	1:A:143:GLN:HG3	2.50	0.41
1:C:2222:ARG:HA	1:C:2223:PRO:HD3	1.85	0.41
1:C:2291[A]:GLU:HG2	1:C:2293:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:HD12	1:A:294:LYS:HG3	2.02	0.41
2:B:720:ALA:HB3	5:B:1110:SF4:S1	2.60	0.41
2:B:834:GLU:HB3	2:B:835:PRO:HA	2.03	0.41
1:A:231:GLY:HA2	1:A:237:ILE:HD12	2.02	0.41
1:A:330:GLN:HB3	1:A:331:PRO:HA	2.03	0.41
1:C:2262:ILE:HD13	1:C:2392:PRO:HA	2.03	0.41
1:C:2448:PHE:HB3	3:C:3000:FAD:N1	2.36	0.41
1:A:72:ALA:HA	1:A:148:ILE:HG12	2.02	0.41
1:A:284:ALA:HA	1:A:333:TYR:O	2.21	0.41
1:C:2507:VAL:CG1	2:B:704:PHE:HB3	2.50	0.41
2:D:2725:CYS:HA	2:D:2726:PRO:HD3	1.81	0.41
2:D:2754:VAL:HG22	2:D:2762:ILE:HG22	2.02	0.41
1:A:29:GLY:O	1:A:34:GLY:HA3	2.21	0.41
1:A:62:ARG:CG	2:B:724:ILE:HD11	2.51	0.41
1:A:291:GLU:HB3	1:A:294:LYS:HD3	2.03	0.41
1:C:2070:LEU:HA	1:C:2365[B]:MET:HB3	2.03	0.41
1:C:2421:PHE:HA	1:C:2422:PRO:HD3	1.93	0.41
2:B:812[B]:ILE:HD13	6:B:5491:HOH:O	2.20	0.41
1:C:2032:PHE:CE1	1:C:2066:VAL:HG21	2.56	0.40
2:B:813:GLN:HA	2:B:814:PRO:HD2	1.84	0.40
1:A:490:ALA:N	1:A:491:PRO:CD	2.84	0.40
1:A:32:PHE:CE1	1:A:66:VAL:HG21	2.57	0.40
1:A:128:LEU:HA	1:A:129:PRO:HD3	1.95	0.40
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.90	0.40
1:C:2314:THR:N	1:C:2315:PRO:HD2	2.36	0.40
2:B:713:CYS:CA	2:B:716:LEU:HD11	2.51	0.40
2:D:2827:LYS:HA	2:D:2827:LYS:HD3	1.88	0.40
1:A:232:ARG:HD2	2:B:767:TYR:HE1	1.86	0.40
1:C:2105:ARG:HD2	1:C:2417:TYR:CE1	2.56	0.40
2:B:794:ASN:HD21	2:B:796:LYS:CB	2.35	0.40
2:D:2813:GLN:HA	2:D:2814:PRO:HD2	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	646/643 (100%)	624 (97%)	22 (3%)	0	100	100
1	C	646/643 (100%)	626 (97%)	20 (3%)	0	100	100
2	B	149/150 (99%)	137 (92%)	9 (6%)	3 (2%)	7	3
2	D	148/150 (99%)	139 (94%)	6 (4%)	3 (2%)	7	3
All	All	1589/1586 (100%)	1526 (96%)	57 (4%)	6 (0%)	34	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	714	LYS
2	B	759	GLN
2	D	2758	PRO
2	D	2759	GLN
2	B	758	PRO
2	D	2734	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	531/526 (101%)	518 (98%)	13 (2%)	49	51
1	C	531/526 (101%)	520 (98%)	11 (2%)	53	57
2	B	131/130 (101%)	126 (96%)	5 (4%)	33	31
2	D	130/130 (100%)	128 (98%)	2 (2%)	65	69
All	All	1323/1312 (101%)	1292 (98%)	31 (2%)	49	53

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	135	ASP

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Mol	Chain	Res	Type
1	A	153	TYR
1	A	257	PHE
1	A	260	ARG
1	A	299	GLU
1	A	301	GLU
1	A	318	ASN
1	A	395	MET
1	A	426	ASN
1	A	444	ASN
1	A	499	LYS
1	A	539	ASN
1	C	2007	LYS
1	C	2153	TYR
1	C	2165	VAL
1	C	2257	PHE
1	C	2260	ARG
1	C	2286	ASN
1	C	2318	ASN
1	C	2395	MET
1	C	2415	GLU
1	C	2444	ASN
1	C	2624	GLU
2	B	713	CYS
2	B	716	LEU
2	B	769	ASP
2	B	785	ASP
2	B	794	ASN
2	D	2758	PRO
2	D	2769	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	115	HIS
1	A	149	HIS
1	A	259	HIS
1	A	310	GLN
1	A	318	ASN
1	A	381	GLN
1	A	383	GLN
1	A	426	ASN

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Mol	Chain	Res	Type
1	A	497	GLN
1	A	539	ASN
1	A	576	HIS
1	C	2068	GLN
1	C	2115	HIS
1	C	2259	HIS
1	C	2286	ASN
1	C	2310	GLN
1	C	2318	ASN
1	C	2369	GLN
1	C	2381	GLN
1	C	2383	GLN
1	C	2497	GLN
1	C	2584	HIS
2	B	794	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
4	ADX	C	3200[B]	-	25,29,29	1.45	5 (20%)	26,45,45	1.30	2 (7%)
5	SF4	D	3100	2	0,12,12	-	-	-		
4	ADX	C	1200[B]	-	25,29,29	1.41	3 (12%)	26,45,45	1.34	3 (11%)
5	SF4	B	1100	2	0,12,12	-	-	-		
5	SF4	D	3110	-	0,12,12	-	-	-		
3	FAD	A	1000	-	53,58,58	5.05	36 (67%)	68,89,89	2.35	27 (39%)
5	SF4	B	1110	-	0,12,12	-	-	-		
4	ADX	C	3200[A]	-	25,29,29	1.32	4 (16%)	26,45,45	1.34	1 (3%)
3	FAD	C	3000	-	53,58,58	4.78	36 (67%)	68,89,89	2.41	25 (36%)
4	ADX	C	1200[A]	-	25,29,29	1.26	3 (12%)	26,45,45	1.36	3 (11%)

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
4	ADX	C	3200[B]	-	-	2/6/32/32	0/3/3/3
5	SF4	D	3100	2	-	-	0/6/5/5
4	ADX	C	1200[B]	-	-	0/6/32/32	0/3/3/3
5	SF4	B	1100	2	-	-	0/6/5/5
5	SF4	D	3110	-	-	-	0/6/5/5
3	FAD	A	1000	-	-	2/30/50/50	0/6/6/6
5	SF4	B	1110	-	-	-	0/6/5/5
4	ADX	C	3200[A]	-	-	0/6/32/32	0/3/3/3
3	FAD	C	3000	-	-	1/30/50/50	0/6/6/6
4	ADX	C	1200[A]	-	-	0/6/32/32	0/3/3/3

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	FAD	C1'-N10	-10.59	1.21	1.48
3	A	1000	FAD	C2B-C1B	10.36	1.69	1.53
3	A	1000	FAD	C8-C7	9.85	1.65	1.40
3	A	1000	FAD	C9A-C5X	9.80	1.57	1.41
3	C	3000	FAD	C1'-N10	-9.75	1.23	1.48
3	C	3000	FAD	C9-C9A	9.71	1.55	1.39
3	A	1000	FAD	C5'-C4'	9.50	1.65	1.51
3	C	3000	FAD	C8-C7	9.41	1.64	1.40
3	C	3000	FAD	C5'-C4'	9.40	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	FAD	C4A-N3A	9.36	1.48	1.35
3	C	3000	FAD	C2B-C1B	9.28	1.67	1.53
3	C	3000	FAD	C9A-C5X	9.15	1.56	1.41
3	C	3000	FAD	C4A-N3A	8.97	1.48	1.35
3	A	1000	FAD	C9-C9A	8.95	1.54	1.39
3	C	3000	FAD	C9A-N10	8.93	1.56	1.41
3	A	1000	FAD	C9A-N10	8.81	1.56	1.41
3	A	1000	FAD	C4X-N5	8.01	1.46	1.30
3	C	3000	FAD	C4X-N5	7.34	1.45	1.30
3	A	1000	FAD	O2B-C2B	6.84	1.59	1.43
3	A	1000	FAD	PA-O1A	-6.81	1.26	1.50
3	A	1000	FAD	C10-N10	6.43	1.51	1.37
3	A	1000	FAD	C2A-N3A	6.23	1.42	1.32
3	A	1000	FAD	C2'-C3'	6.16	1.65	1.53
3	C	3000	FAD	O2B-C2B	6.01	1.57	1.43
3	A	1000	FAD	O4B-C1B	5.91	1.49	1.41
3	C	3000	FAD	C4-N3	5.87	1.49	1.38
3	C	3000	FAD	C10-N10	5.84	1.50	1.37
3	A	1000	FAD	C6-C7	5.65	1.47	1.39
3	C	3000	FAD	C2A-N3A	5.31	1.40	1.32
3	C	3000	FAD	C2'-C3'	5.28	1.63	1.53
3	A	1000	FAD	C2A-N1A	5.13	1.43	1.33
3	C	3000	FAD	C6-C5X	5.10	1.48	1.40
3	C	3000	FAD	O4B-C1B	5.01	1.48	1.41
3	A	1000	FAD	C10-N1	4.90	1.43	1.33
3	A	1000	FAD	O3'-C3'	-4.89	1.31	1.43
3	C	3000	FAD	C9-C8	4.72	1.46	1.39
3	A	1000	FAD	C6-C5X	4.60	1.47	1.40
3	C	3000	FAD	O3'-C3'	-4.56	1.32	1.43
3	C	3000	FAD	PA-O1A	-4.46	1.35	1.50
3	A	1000	FAD	C4-N3	4.44	1.47	1.38
3	C	3000	FAD	C10-N1	4.27	1.42	1.33
3	C	3000	FAD	O2'-C2'	-4.20	1.34	1.43
3	C	3000	FAD	C6-C7	4.18	1.45	1.39
3	C	3000	FAD	C4X-C10	3.97	1.55	1.44
3	A	1000	FAD	C4X-C10	3.91	1.55	1.44
3	A	1000	FAD	C3B-C4B	3.85	1.62	1.53
4	C	1200[B]	ADX	PA-O3A	3.74	1.62	1.59
4	C	3200[B]	ADX	PA-O3A	3.74	1.62	1.59
3	A	1000	FAD	C8A-N7A	-3.68	1.28	1.34
3	C	3000	FAD	C3B-C4B	3.61	1.62	1.53
3	C	3000	FAD	C2A-N1A	3.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3000	FAD	O2-C2	-3.27	1.18	1.24
3	A	1000	FAD	O2'-C2'	-3.12	1.36	1.43
4	C	1200[A]	ADX	PA-O3A	2.99	1.61	1.59
3	A	1000	FAD	C9-C8	2.95	1.43	1.39
3	A	1000	FAD	C4'-C3'	-2.93	1.47	1.53
3	A	1000	FAD	C5A-C4A	2.82	1.48	1.40
3	C	3000	FAD	C8A-N7A	-2.82	1.29	1.34
3	A	1000	FAD	C2-N3	2.80	1.45	1.39
4	C	3200[A]	ADX	PA-O3A	2.78	1.61	1.59
4	C	3200[B]	ADX	C2-N1	2.76	1.39	1.33
3	A	1000	FAD	PA-O5B	2.73	1.70	1.59
4	C	3200[A]	ADX	C2-N1	2.72	1.39	1.33
3	C	3000	FAD	C5X-N5	2.65	1.44	1.39
3	C	3000	FAD	C5A-C4A	2.52	1.47	1.40
3	C	3000	FAD	PA-O2A	-2.48	1.43	1.55
3	C	3000	FAD	P-O1P	-2.45	1.42	1.50
4	C	3200[B]	ADX	C5-N7	-2.42	1.30	1.39
4	C	3200[A]	ADX	C5-N7	-2.41	1.31	1.39
3	C	3000	FAD	PA-O5B	2.38	1.68	1.59
3	C	3000	FAD	C2-N3	2.37	1.44	1.39
3	A	1000	FAD	C2B-C3B	2.37	1.59	1.53
4	C	1200[B]	ADX	C2-N1	2.34	1.38	1.33
4	C	1200[A]	ADX	C2-N1	2.34	1.38	1.33
3	A	1000	FAD	C8M-C8	-2.32	1.46	1.51
4	C	3200[B]	ADX	O4'-C1'	2.31	1.44	1.41
3	A	1000	FAD	C6A-N1A	2.30	1.47	1.37
4	C	3200[A]	ADX	O4'-C1'	2.25	1.44	1.41
3	A	1000	FAD	C5X-N5	2.22	1.43	1.39
4	C	1200[B]	ADX	C5-N7	-2.22	1.31	1.39
4	C	1200[A]	ADX	C5-N7	-2.21	1.31	1.39
4	C	3200[B]	ADX	PA-O2A	-2.16	1.45	1.55
3	C	3000	FAD	O5B-C5B	-2.10	1.36	1.44
3	C	3000	FAD	C6A-N1A	2.06	1.46	1.37
3	A	1000	FAD	P-O2P	2.04	1.64	1.55
3	A	1000	FAD	C5B-C4B	2.02	1.57	1.51
3	C	3000	FAD	P-O2P	2.01	1.64	1.55

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3000	FAD	O4B-C4B-C3B	6.73	118.43	105.11
3	C	3000	FAD	O4B-C1B-C2B	-6.48	97.46	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3000	FAD	C3B-C2B-C1B	6.45	110.69	100.98
3	A	1000	FAD	O4B-C4B-C3B	6.44	117.86	105.11
3	A	1000	FAD	O4B-C1B-C2B	-5.98	98.18	106.93
3	C	3000	FAD	C2B-C3B-C4B	-5.84	91.30	102.64
4	C	3200[B]	ADX	N3-C2-N1	-5.41	120.22	128.68
4	C	3200[A]	ADX	N3-C2-N1	-5.40	120.25	128.68
3	A	1000	FAD	C2B-C3B-C4B	-5.20	92.53	102.64
4	C	1200[A]	ADX	N3-C2-N1	-4.93	120.97	128.68
4	C	1200[B]	ADX	N3-C2-N1	-4.92	120.99	128.68
3	A	1000	FAD	C3B-C2B-C1B	4.73	108.10	100.98
3	A	1000	FAD	C10-N1-C2	4.33	125.57	116.90
3	C	3000	FAD	C9-C9A-N10	4.00	127.24	121.84
3	A	1000	FAD	O4'-C4'-C3'	3.84	118.45	109.10
3	C	3000	FAD	C10-N1-C2	3.82	124.53	116.90
3	C	3000	FAD	P-O3P-PA	-3.67	120.24	132.83
3	C	3000	FAD	O4'-C4'-C3'	3.62	117.89	109.10
3	C	3000	FAD	O2B-C2B-C1B	-3.61	97.53	110.85
3	C	3000	FAD	O3'-C3'-C4'	3.52	117.31	108.81
3	A	1000	FAD	C9-C9A-N10	3.52	126.59	121.84
3	A	1000	FAD	P-O3P-PA	-3.48	120.88	132.83
3	A	1000	FAD	O2B-C2B-C1B	-3.38	98.38	110.85
3	A	1000	FAD	C4-C4X-N5	3.35	123.00	118.23
3	C	3000	FAD	O2'-C2'-C3'	3.33	117.20	109.10
3	A	1000	FAD	O2'-C2'-C3'	3.32	117.18	109.10
3	A	1000	FAD	C6-C5X-C9A	3.30	123.61	118.94
3	A	1000	FAD	N3A-C2A-N1A	-3.27	123.57	128.68
3	C	3000	FAD	C6-C5X-C9A	3.26	123.56	118.94
3	A	1000	FAD	O3'-C3'-C4'	3.19	116.53	108.81
3	C	3000	FAD	C9-C9A-C5X	-3.05	114.35	120.11
3	A	1000	FAD	C5B-C4B-C3B	-2.78	104.75	115.18
3	C	3000	FAD	N3A-C2A-N1A	-2.74	124.39	128.68
3	A	1000	FAD	C9-C9A-C5X	-2.68	115.05	120.11
3	A	1000	FAD	O5'-P-O1P	-2.66	98.68	109.07
3	C	3000	FAD	O5'-P-O1P	-2.60	98.91	109.07
3	A	1000	FAD	PA-O5B-C5B	2.54	136.59	121.68
3	C	3000	FAD	C4-C4X-N5	2.51	121.80	118.23
3	A	1000	FAD	N6A-C6A-N1A	2.50	123.76	118.57
4	C	1200[B]	ADX	O4'-C4'-C5'	2.40	117.27	109.37
3	C	3000	FAD	C9A-C9-C8	2.39	124.12	119.30
3	A	1000	FAD	O2B-C2B-C3B	2.39	119.56	111.82
3	A	1000	FAD	C9A-C9-C8	2.38	124.09	119.30
3	A	1000	FAD	C4X-C10-N10	2.37	119.94	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1000	FAD	C4X-C10-N1	-2.35	119.27	124.73
3	C	3000	FAD	N6A-C6A-N1A	2.35	123.45	118.57
3	C	3000	FAD	PA-O5B-C5B	2.33	135.37	121.68
3	C	3000	FAD	C4X-C10-N10	2.33	119.89	116.48
3	C	3000	FAD	C5B-C4B-C3B	-2.27	106.67	115.18
3	C	3000	FAD	O4'-C4'-C5'	-2.24	104.89	109.92
3	C	3000	FAD	C6-C5X-N5	-2.22	114.64	118.51
4	C	1200[B]	ADX	C4-C5-N7	-2.19	107.11	109.40
4	C	1200[A]	ADX	C4-C5-N7	-2.19	107.12	109.40
3	A	1000	FAD	C5'-C4'-C3'	-2.18	107.99	112.20
3	A	1000	FAD	C6-C5X-N5	-2.17	114.73	118.51
4	C	1200[A]	ADX	O4'-C4'-C5'	2.13	116.38	109.37
3	C	3000	FAD	C4X-C10-N1	-2.11	119.83	124.73
3	A	1000	FAD	C5A-C6A-N6A	-2.10	117.17	120.35
3	C	3000	FAD	O2A-PA-O1A	2.07	122.49	112.24
3	A	1000	FAD	C5X-N5-C4X	2.01	121.42	118.07
4	C	3200[B]	ADX	C2'-C3'-C4'	-2.00	98.75	102.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3200[B]	ADX	C5'-O5'-PA-O3A
4	C	3200[B]	ADX	C5'-O5'-PA-O2A
3	A	1000	FAD	N10-C1'-C2'-O2'
3	C	3000	FAD	O4B-C4B-C5B-O5B
3	A	1000	FAD	O4B-C4B-C5B-O5B

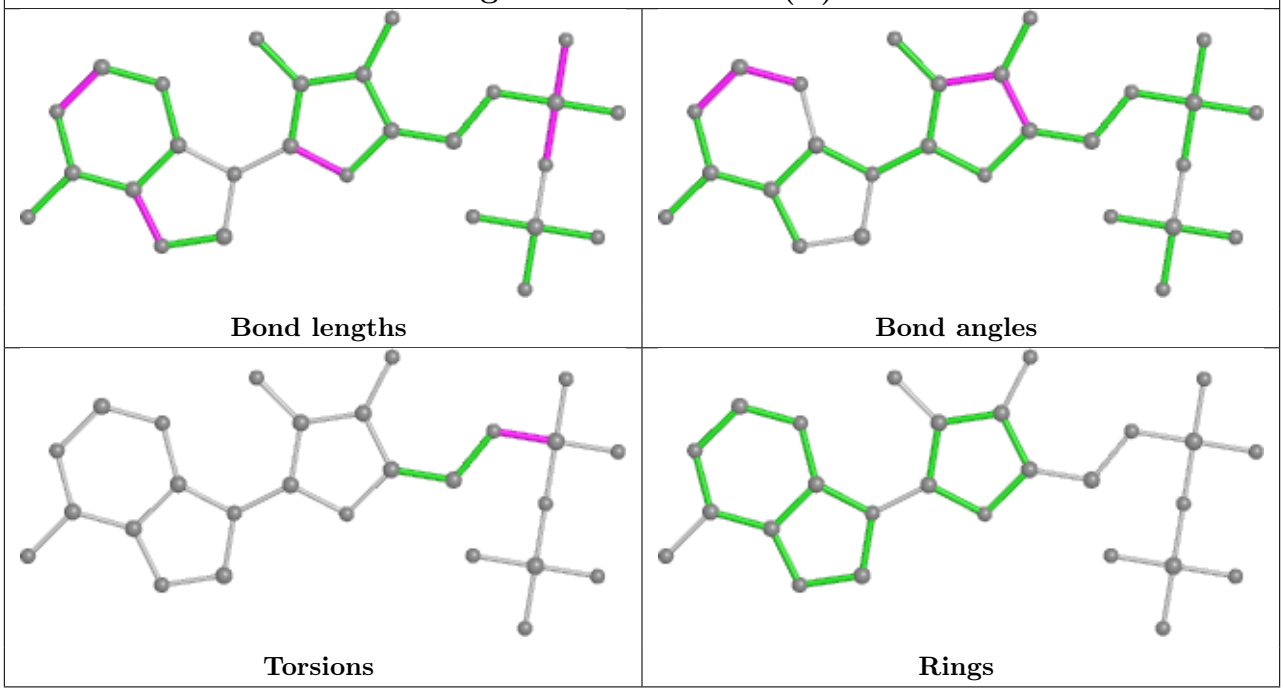
There are no ring outliers.

8 monomers are involved in 25 short contacts:

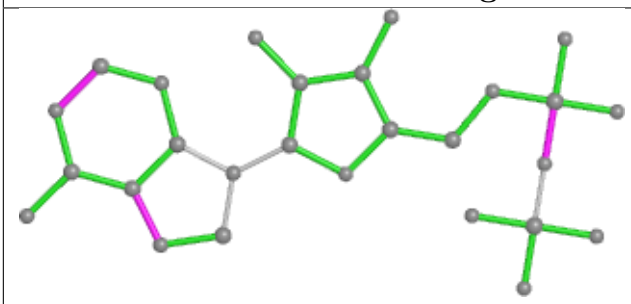
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3200[B]	ADX	6	0
4	C	1200[B]	ADX	6	0
5	D	3110	SF4	3	0
3	A	1000	FAD	2	0
5	B	1110	SF4	1	0
4	C	3200[A]	ADX	2	0
3	C	3000	FAD	4	0
4	C	1200[A]	ADX	1	0

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

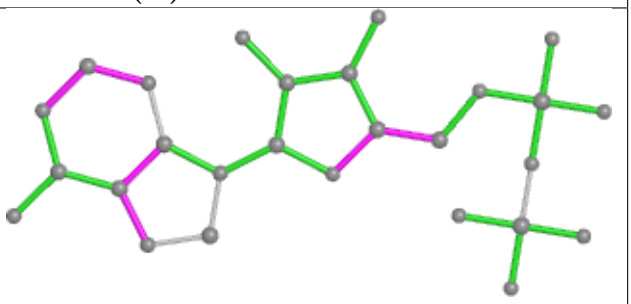
Ligand ADX C 3200 (B)



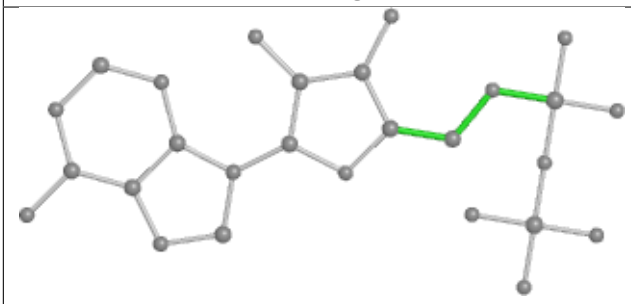
Ligand ADX C 1200 (B)



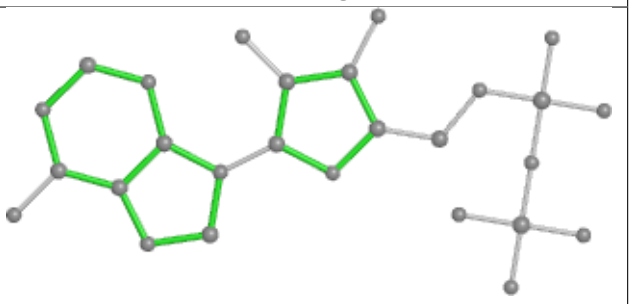
Bond lengths



Bond angles

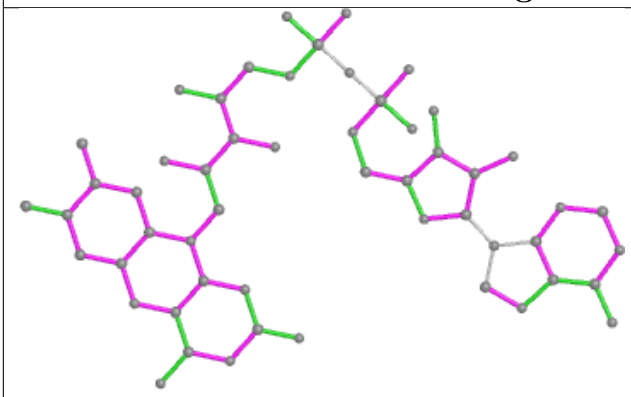


Torsions

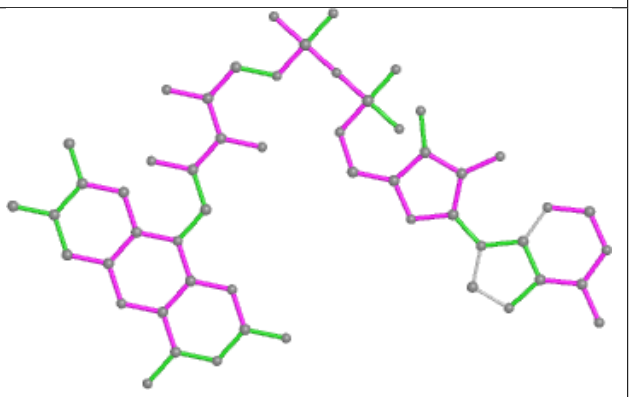


Rings

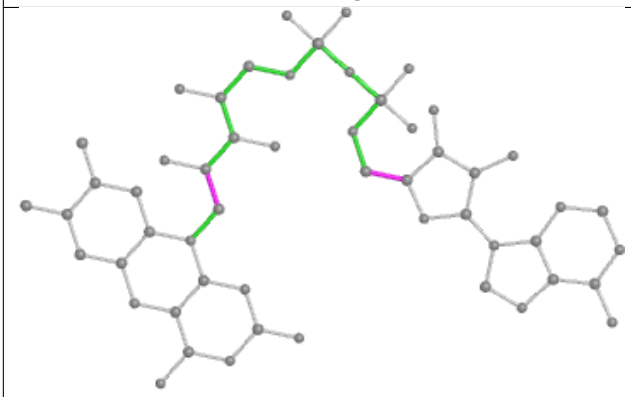
Ligand FAD A 1000



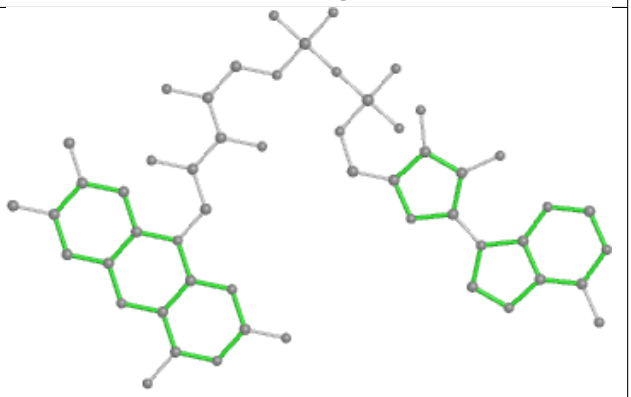
Bond lengths



Bond angles

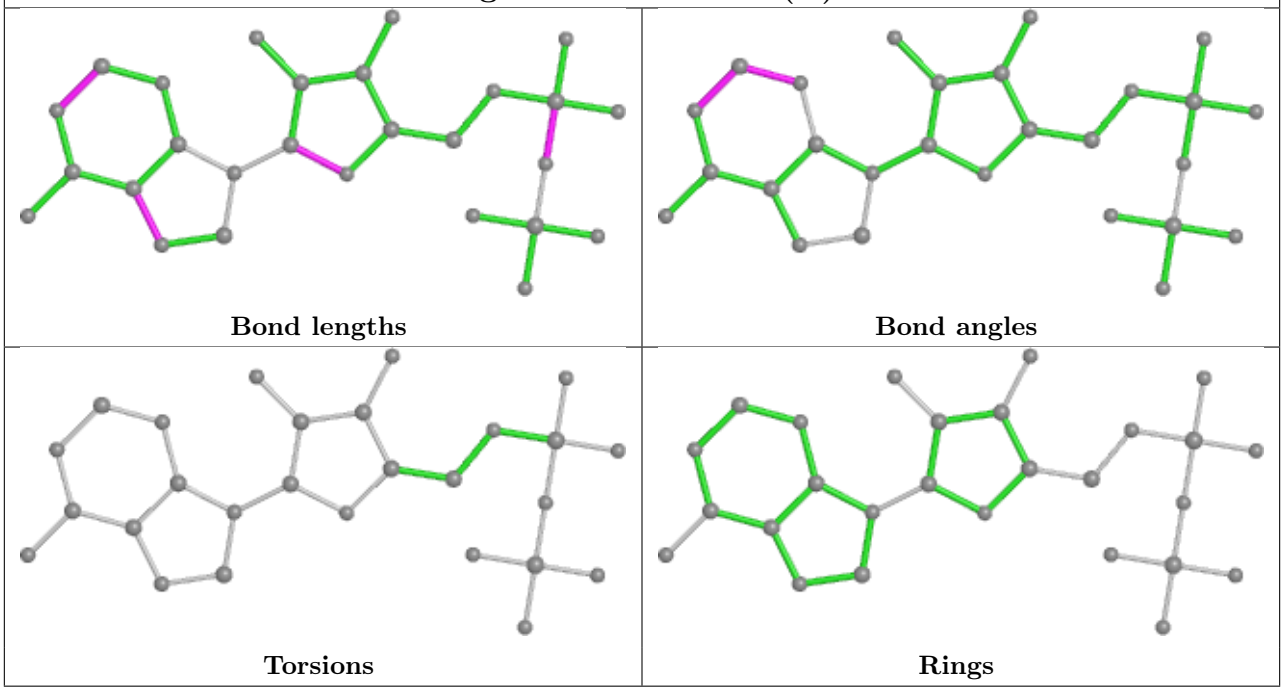


Torsions

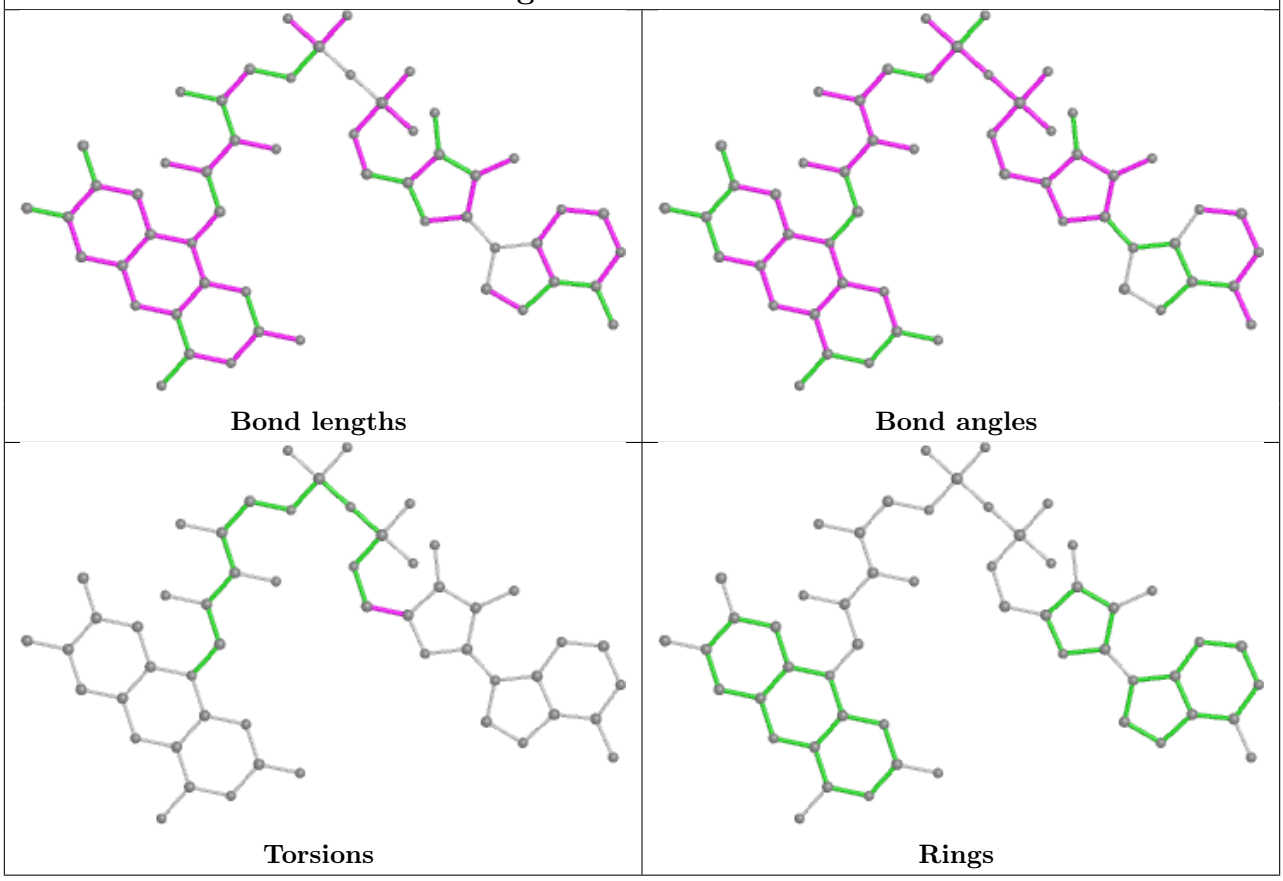


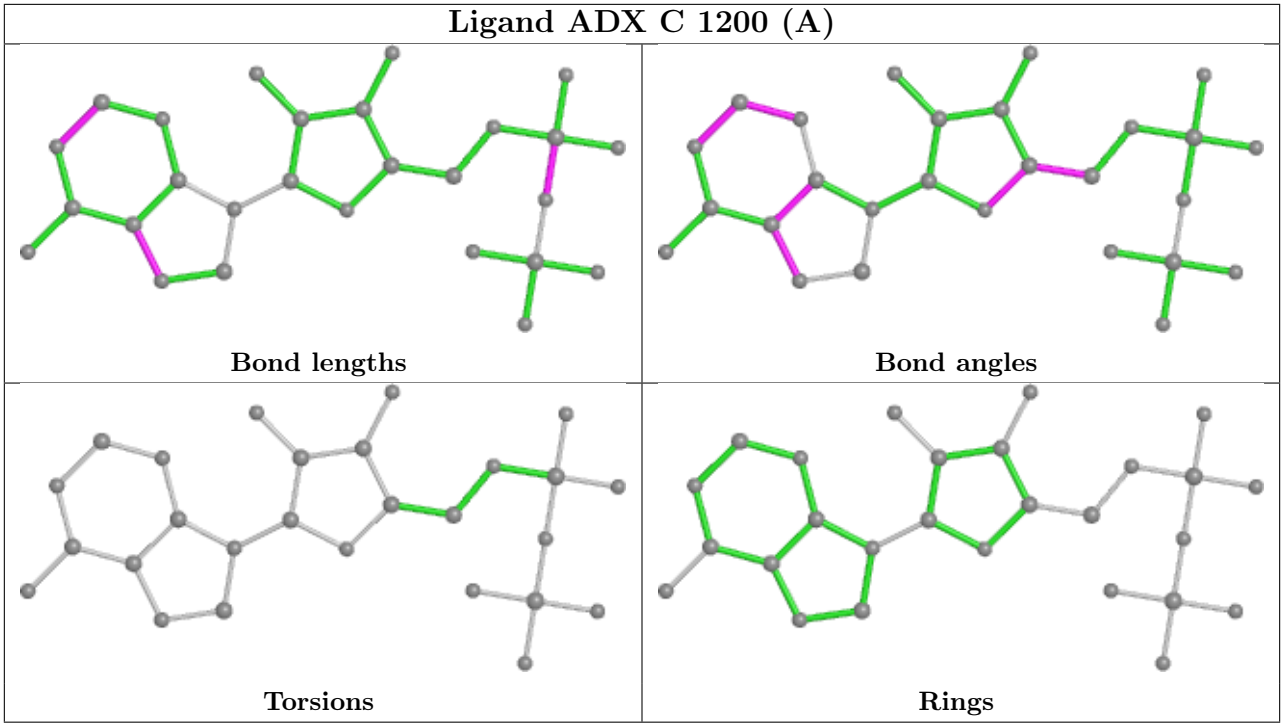
Rings

Ligand ADX C 3200 (A)



Ligand FAD C 3000





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.