



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2025 – 11:53 am BST

PDB ID : 7APR / pdb_00007apr
Title : Bacillithiol Disulfide Reductase Bdr (YpdA) from Staphylococcus aureus
Authors : Hammerstad, M.; Hersleth, H.-P.
Deposited on : 2020-10-19
Resolution : 3.10 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

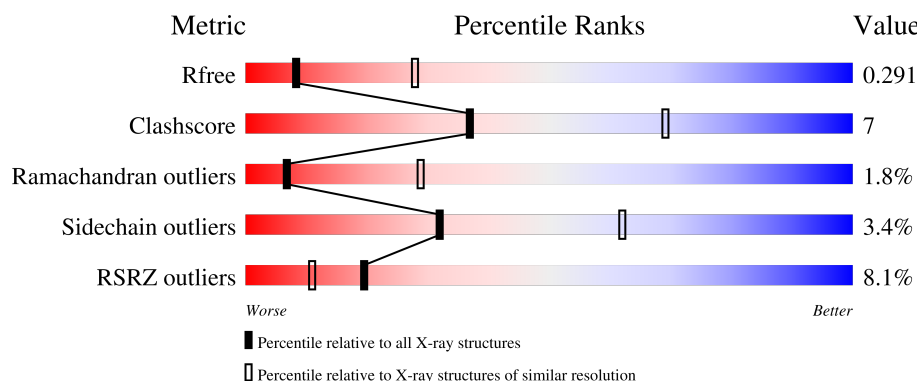
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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	328	<div> <div>2%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	B	328	<div> <div>%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	C	328	<div> <div>%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	D	328	<div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	E	328	<div> <div>%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	328	<div><div><div>%</div><div><div></div><div>80%</div><div>16%</div><div></div><div></div></div></div></div>
1	G	328	<div><div><div>28%</div><div><div></div><div>61%</div><div>27%</div><div></div><div></div></div></div><div><div></div><div></div><div>11%</div><div></div></div></div>
1	H	328	<div><div><div>30%</div><div><div></div><div>69%</div><div>23%</div><div></div><div></div></div></div><div><div></div><div></div><div>5%</div><div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20960 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 YpdA family putative bacillithiol disulfide reductase Bdr.

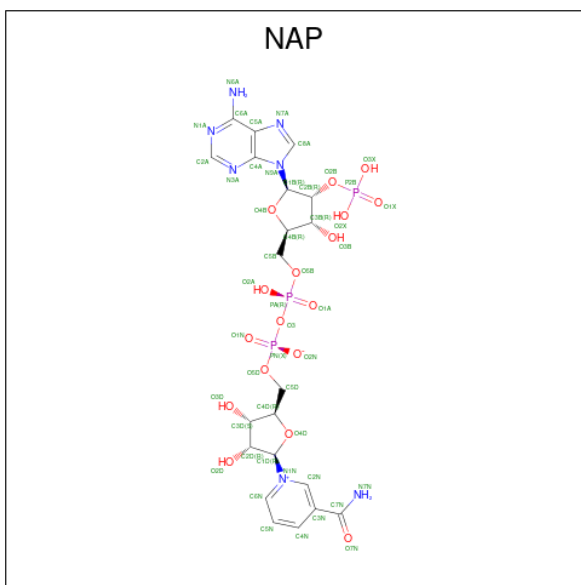
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	3	0
			2582	1650	427	496	9			
1	B	322	Total	C	N	O	S	0	1	0
			2555	1634	421	491	9			
1	C	323	Total	C	N	O	S	0	4	0
			2593	1661	426	497	9			
1	D	323	Total	C	N	O	S	0	2	0
			2575	1648	424	494	9			
1	E	323	Total	C	N	O	S	0	2	0
			2569	1642	424	494	9			
1	F	323	Total	C	N	O	S	0	3	0
			2576	1649	421	497	9			
1	G	293	Total	C	N	O	S	0	0	0
			2308	1473	378	449	8			
1	H	318	Total	C	N	O	S	0	0	0
			2514	1607	412	486	9			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 96	C 42	N 14	O 34	P 6	0	1
3	F	1	Total 96	C 42	N 14	O 34	P 6	0	1

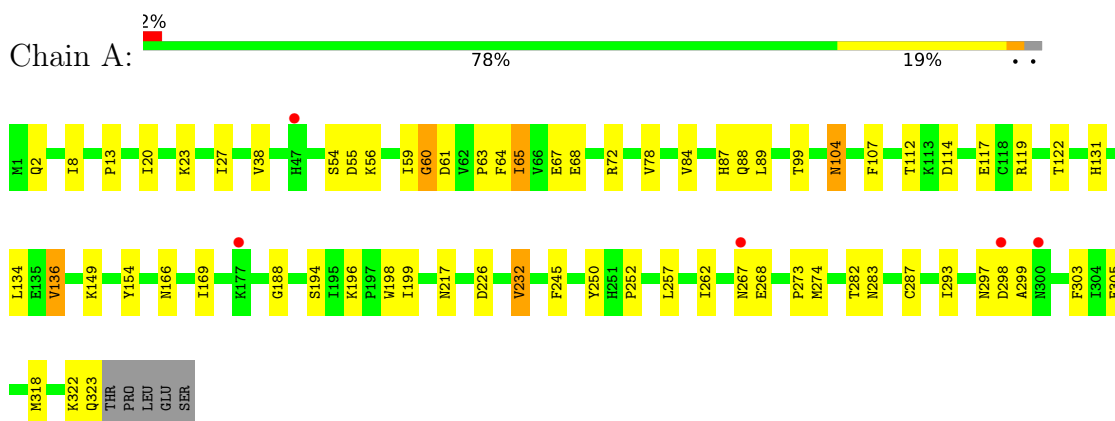
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	C	4	Total O 4 4	0	0
4	D	5	Total O 5 5	0	0
4	E	4	Total O 4 4	0	0
4	F	4	Total O 4 4	0	0
4	G	2	Total O 2 2	0	0
4	H	1	Total O 1 1	0	0

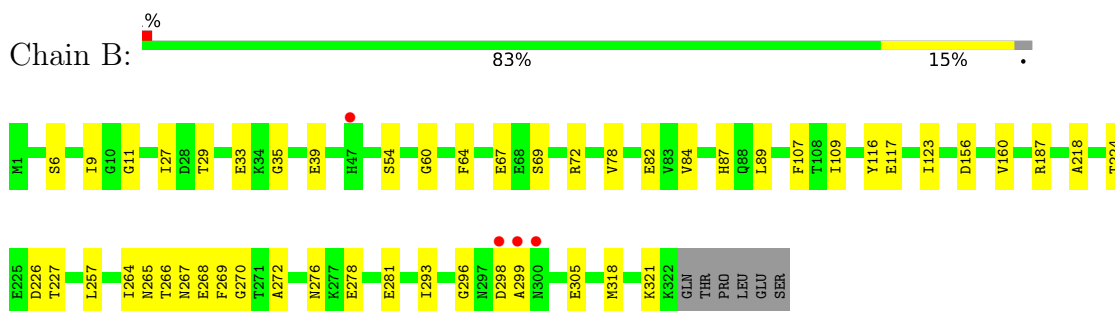
3 Residue-property plots [i](#)

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.

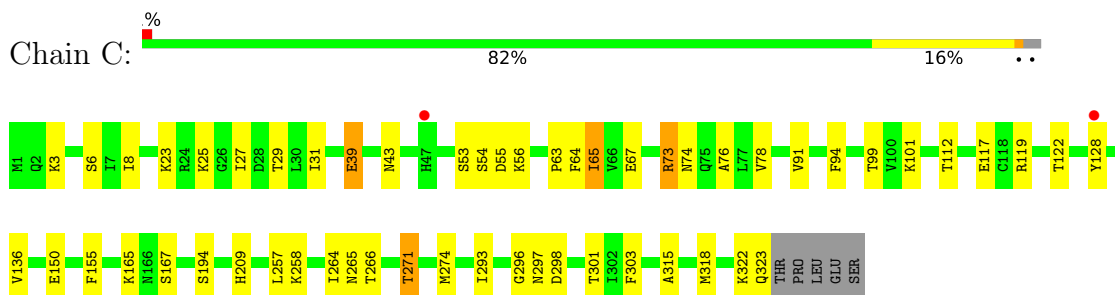
- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr



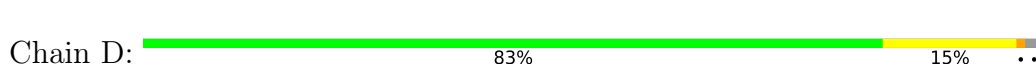
- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

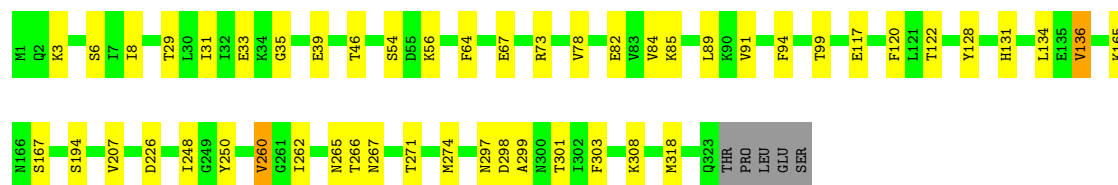


- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

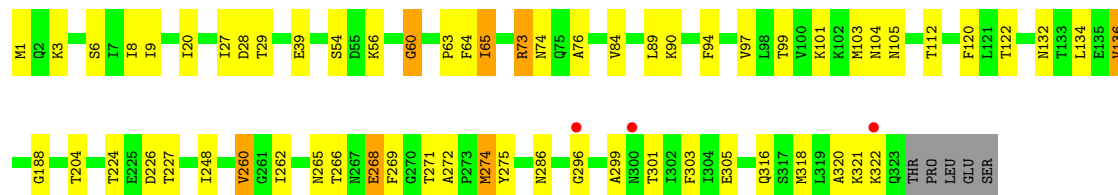
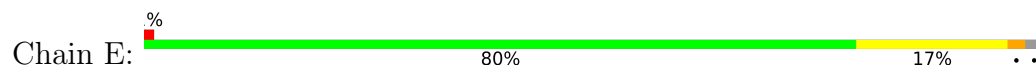


- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

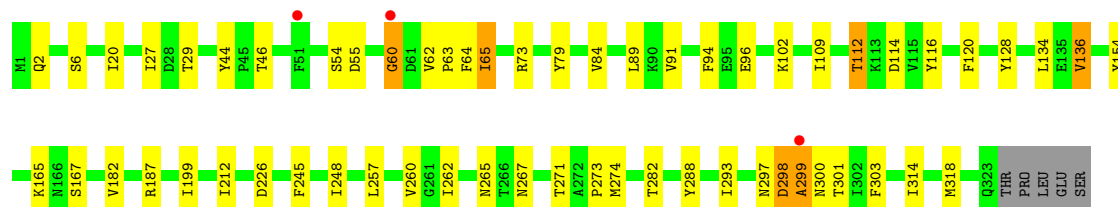




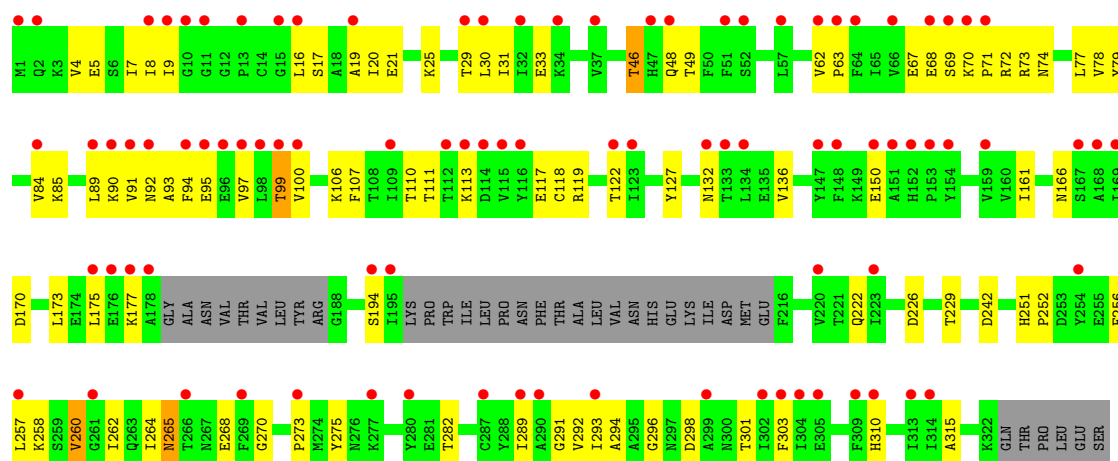
- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr



- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

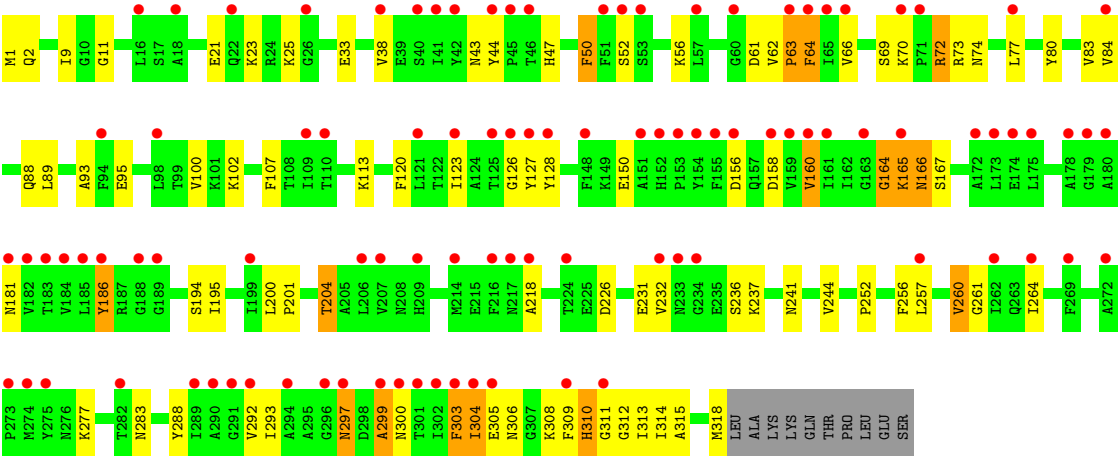


- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr



- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	180.31Å 180.31Å 350.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.94 – 3.10 29.94 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.94-3.10) 99.8 (29.94-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 3.11Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, REFMAC 5.8.0253	Depositor
R, R_{free}	0.244 , 0.291 0.245 , 0.291	Depositor DCC
R_{free} test set	3107 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20960	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, 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	0.13	0/2639	0.39	0/3575
1	B	0.13	0/2612	0.34	0/3540
1	C	0.13	0/2655	0.36	0/3598
1	D	0.13	0/2633	0.36	0/3568
1	E	0.13	0/2629	0.37	0/3563
1	F	0.12	0/2639	0.37	0/3576
1	G	0.19	1/2355 (0.0%)	0.47	0/3185
1	H	0.14	0/2570	0.43	0/3485
All	All	0.14	1/20732 (0.0%)	0.39	0/28090

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	113	LYS	CA-C	-5.43	1.49	1.52

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	2582	0	2531	41	0
1	B	2555	0	2504	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2593	0	2536	32	0
1	D	2575	0	2520	29	0
1	E	2569	0	2518	28	0
1	F	2576	0	2524	33	0
1	G	2308	0	2256	60	0
1	H	2514	0	2456	56	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	3	0
2	D	53	0	31	1	0
2	E	53	0	31	0	0
2	F	53	0	31	2	0
2	G	53	0	31	0	0
2	H	53	0	31	3	0
3	C	48	0	23	1	0
3	D	96	0	50	6	0
3	F	96	0	50	8	0
4	A	4	0	0	0	0
4	C	4	0	0	0	0
4	D	5	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
All	All	20960	0	20216	288	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 7.

All (288) 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:H:21:GLU:HG3	1:H:310:HIS:HB3	1.57	0.84
1:A:297:ASN:O	1:A:299:ALA:N	2.14	0.80
1:C:301:THR:HG23	1:E:188:GLY:HA2	1.68	0.75
1:D:299:ALA:O	3:D:402[A]:NAP:O2D	2.06	0.73
1:H:84:VAL:HG13	1:H:89:LEU:HB2	1.71	0.72
1:H:261:GLY:O	1:H:283:ASN:ND2	2.19	0.72
1:H:292:VAL:HG13	1:H:304:ILE:HD12	1.71	0.71
1:E:272:ALA:HB2	1:E:296:GLY:HA3	1.71	0.71
1:G:265:ASN:HB3	1:G:268:GLU:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:ILE:HD13	1:F:318:MET:HE2	1.74	0.69
1:A:63:PRO:HB2	1:A:65:ILE:HD12	1.75	0.69
1:E:20:ILE:HD13	1:E:60:GLY:HA3	1.74	0.69
1:G:7:ILE:HG12	1:G:30:LEU:HD23	1.75	0.69
1:C:266:THR:HG21	1:E:271:THR:H	1.58	0.69
1:G:74:ASN:HA	1:G:77:LEU:HB3	1.75	0.69
1:G:73:ARG:NH2	1:H:150:GLU:OE2	2.21	0.68
1:A:134:LEU:HG	1:A:136:VAL:HG13	1.76	0.67
1:D:84:VAL:HG13	1:D:89:LEU:HB2	1.76	0.67
1:H:52:SER:HB3	1:H:56:LYS:HB2	1.77	0.67
1:H:311:GLY:O	1:H:313:ILE:N	2.27	0.66
1:D:120:PHE:HB3	1:D:318:MET:HE2	1.77	0.66
1:E:28:ASP:OD1	1:E:90:LYS:NZ	2.29	0.66
1:G:8:ILE:N	1:G:30:LEU:O	2.29	0.66
1:H:100:VAL:HB	1:H:260:VAL:HG12	1.78	0.66
1:H:44:TYR:HH	2:H:401:FAD:HO2'	1.37	0.65
1:H:165:LYS:O	1:H:167:SER:N	2.25	0.65
1:B:109:ILE:HB	1:B:116:TYR:HB2	1.78	0.65
1:E:134:LEU:HG	1:E:136:VAL:HG13	1.78	0.65
1:C:27:ILE:HD13	1:C:318:MET:HE2	1.78	0.64
1:F:165:LYS:HD2	3:F:402[B]:NAP:H3B	1.78	0.64
1:H:62:VAL:HG21	1:H:83:VAL:HG22	1.80	0.64
1:G:9:ILE:HD13	1:G:97:VAL:HG11	1.79	0.63
1:G:70:LYS:C	1:G:72:ARG:H	2.07	0.63
1:A:119:ARG:HH12	1:A:323:GLN:HA	1.62	0.63
1:C:258:LYS:HE3	1:C:264:ILE:HD12	1.79	0.63
1:E:63:PRO:HB2	1:E:65:ILE:HD12	1.81	0.63
1:A:27:ILE:HD13	1:A:318:MET:HE2	1.79	0.62
1:A:67:GLU:HA	1:D:78:VAL:HG21	1.81	0.62
1:G:31:ILE:O	1:G:91:VAL:HA	1.99	0.61
1:A:65:ILE:HG12	1:D:82:GLU:HG3	1.82	0.61
1:G:99:THR:HB	1:G:110:THR:HB	1.81	0.61
1:A:188:GLY:HA2	1:F:301:THR:HG23	1.83	0.61
1:F:134:LEU:HG	1:F:136:VAL:HG13	1.84	0.60
1:G:166:ASN:ND2	1:G:194:SER:O	2.34	0.60
1:G:132:ASN:OD1	1:G:251:HIS:ND1	2.35	0.60
1:B:60:GLY:O	1:B:87:HIS:NE2	2.19	0.59
1:D:128:TYR:OH	2:D:401:FAD:H9	2.02	0.59
1:D:54:SER:OG	1:D:64:PHE:O	2.20	0.59
1:F:265:ASN:HD21	1:F:274:MET:HG3	1.68	0.59
1:F:20:ILE:HD13	1:F:60:GLY:HA3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LYS:HB2	1:A:199:ILE:HD12	1.85	0.59
1:A:56:LYS:HB3	1:A:305:GLU:HG2	1.85	0.59
1:H:1:MET:HG2	1:H:2:GLN:H	1.67	0.58
1:G:62:VAL:HG22	1:G:79:TYR:CE1	2.38	0.58
1:C:265:ASN:ND2	1:C:274:MET:SD	2.76	0.57
1:H:44:TYR:OH	2:H:401:FAD:O2'	2.13	0.57
1:G:25:LYS:HG3	1:G:315:ALA:HB1	1.85	0.57
1:G:298:ASP:OD2	1:G:301:THR:OG1	2.20	0.57
1:G:46:THR:O	1:H:70:LYS:NZ	2.33	0.57
1:H:72:ARG:HG3	1:H:74:ASN:H	1.68	0.57
1:D:165:LYS:HD2	3:D:402[B]:NAP:H3B	1.87	0.56
1:E:27:ILE:HD13	1:E:318:MET:HE2	1.87	0.56
1:F:154:TYR:CE2	1:F:245:PHE:HZ	2.23	0.56
1:G:46:THR:HG23	1:G:73:ARG:HH21	1.70	0.56
1:A:20:ILE:HD13	1:A:60:GLY:HA3	1.88	0.56
1:G:8:ILE:HG12	1:G:122:THR:HB	1.88	0.56
1:F:44:TYR:HB2	1:F:73:ARG:HD2	1.88	0.55
1:G:29:THR:O	1:G:90:LYS:HD2	2.05	0.55
1:G:8:ILE:HB	1:G:31:ILE:HG12	1.89	0.55
1:G:5:GLU:HG3	1:G:119:ARG:HD2	1.88	0.55
1:C:53:SER:OG	1:C:55:ASP:OD1	2.21	0.55
1:H:252:PRO:HB3	1:H:293:ILE:HD12	1.89	0.54
1:G:67:GLU:HB2	1:G:78:VAL:HG11	1.90	0.54
1:H:120:PHE:HB3	1:H:318:MET:HE2	1.89	0.54
1:A:297:ASN:C	1:A:299:ALA:H	2.14	0.54
1:G:150:GLU:OE2	1:H:73:ARG:NH2	2.40	0.54
1:C:8:ILE:HG12	1:C:122:THR:HB	1.90	0.54
1:F:84:VAL:HG13	1:F:89:LEU:HB2	1.89	0.54
1:H:56:LYS:HG2	1:H:306:ASN:HD22	1.72	0.54
1:E:56:LYS:HB3	1:E:305:GLU:HG2	1.88	0.54
1:B:257:LEU:HD11	1:B:293:ILE:HD11	1.90	0.54
1:A:154:TYR:CE2	1:A:245:PHE:HZ	2.27	0.53
1:A:78:VAL:HG21	1:D:67:GLU:HA	1.90	0.53
1:G:70:LYS:O	1:G:72:ARG:N	2.40	0.53
1:H:43:ASN:ND2	1:H:128:TYR:OH	2.41	0.53
1:H:300:ASN:OD1	1:H:308:LYS:NZ	2.39	0.53
1:A:104:ASN:OD1	1:A:104:ASN:N	2.42	0.53
1:H:56:LYS:HB3	1:H:306:ASN:HB2	1.89	0.53
1:A:23:LYS:NZ	1:A:88:GLN:O	2.41	0.53
1:H:9:ILE:HD12	1:H:123:ILE:HG12	1.89	0.53
1:G:252:PRO:HB3	1:G:293:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:ILE:HG12	1:E:122:THR:HB	1.90	0.52
1:F:187:ARG:NE	3:F:402[A]:NAP:O2B	2.42	0.52
1:B:9:ILE:HD12	1:B:123:ILE:HG13	1.92	0.52
1:B:6:SER:HB3	1:B:29:THR:HG22	1.92	0.52
1:B:27:ILE:HD13	1:B:318:MET:HE2	1.92	0.51
1:A:262:ILE:HD13	1:A:282:THR:HG21	1.93	0.51
1:C:155:PHE:HE1	1:D:85:LYS:HE3	1.75	0.51
1:G:4:VAL:O	1:G:118:CYS:HA	2.11	0.51
1:D:8:ILE:HG12	1:D:122:THR:HB	1.91	0.51
1:H:73:ARG:HH11	1:H:77:LEU:HD11	1.74	0.51
1:A:54:SER:OG	1:A:64:PHE:O	2.23	0.51
1:H:25:LYS:HG3	1:H:315:ALA:HB1	1.93	0.51
1:C:128[A]:TYR:OH	2:C:401:FAD:H1'1	2.10	0.51
1:G:107:PHE:O	1:G:117:GLU:HA	2.10	0.51
1:A:60:GLY:O	1:A:87:HIS:NE2	2.32	0.50
1:A:274:MET:HE3	1:A:283:ASN:HB3	1.93	0.50
1:A:252:PRO:HB3	1:A:293:ILE:HG13	1.93	0.50
1:E:54:SER:OG	1:E:64:PHE:O	2.28	0.50
1:H:226:ASP:N	1:H:226:ASP:OD1	2.42	0.50
1:A:131:HIS:HA	1:A:250:TYR:HD1	1.77	0.50
1:B:281:GLU:CD	1:B:321:LYS:HZ1	2.20	0.50
1:B:224:THR:HG1	1:B:227:THR:HG1	1.58	0.50
1:H:256:PHE:O	1:H:260:VAL:HG13	2.11	0.49
1:E:73:ARG:O	1:E:76:ALA:N	2.42	0.49
1:C:119:ARG:NH2	1:C:323:GLN:HB3	2.28	0.49
1:B:272:ALA:HB2	1:B:296:GLY:HA3	1.94	0.49
1:D:134:LEU:HG	1:D:136:VAL:HG13	1.95	0.49
1:E:272:ALA:HB2	1:E:296:GLY:CA	2.43	0.49
1:B:226:ASP:OD1	1:B:226:ASP:N	2.45	0.49
1:H:305:GLU:HB2	1:H:308:LYS:HE3	1.95	0.49
1:C:6:SER:HB3	1:C:29:THR:HG22	1.94	0.48
1:A:84:VAL:HG13	1:A:89:LEU:HB2	1.95	0.48
1:F:298:ASP:C	1:F:300:ASN:H	2.22	0.48
1:H:232:VAL:HB	1:H:237:LYS:HE3	1.95	0.48
1:G:72:ARG:NH2	1:H:69:SER:O	2.46	0.48
1:A:257:LEU:HD13	1:A:273:PRO:HG3	1.95	0.48
1:G:33:GLU:O	1:G:94:PHE:HB2	2.13	0.48
1:H:127:TYR:HE2	1:H:303:PHE:HE1	1.62	0.48
1:A:107:PHE:O	1:A:117:GLU:HA	2.14	0.48
1:F:54:SER:OG	1:F:64:PHE:O	2.30	0.48
1:G:70:LYS:HB3	1:G:71:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:NH1	1:D:67:GLU:OE2	2.48	0.47
1:C:3:LYS:HG2	1:C:117:GLU:HB3	1.95	0.47
1:F:63:PRO:HB2	1:F:65:ILE:HD12	1.96	0.47
1:A:257:LEU:HD11	1:A:293:ILE:HD11	1.96	0.47
1:D:3:LYS:HG2	1:D:117:GLU:HB3	1.96	0.47
1:E:268:GLU:HB2	1:E:269:PHE:H	1.54	0.47
1:G:84:VAL:HG22	1:G:89:LEU:HD12	1.96	0.47
1:B:72:ARG:NH2	1:C:67:GLU:OE2	2.47	0.47
1:H:102:LYS:HD3	1:H:107:PHE:CE2	2.49	0.47
1:H:231:GLU:HG2	1:H:236:SER:HA	1.96	0.47
1:C:271:THR:OG1	1:C:297:ASN:OD1	2.33	0.47
1:E:265:ASN:OD1	1:E:274:MET:HE2	2.15	0.47
1:G:19:ALA:HB2	1:G:31:ILE:HD11	1.95	0.47
1:G:275:TYR:OH	1:G:294:ALA:HB1	2.15	0.47
1:B:276:ASN:O	1:B:278:GLU:N	2.42	0.47
1:C:128[A]:TYR:OH	2:C:401:FAD:H9	2.14	0.47
1:E:1:MET:HE3	1:E:3:LYS:HE3	1.96	0.47
1:G:7:ILE:HG13	1:G:118:CYS:HB3	1.97	0.47
1:E:6:SER:HB3	1:E:29:THR:HG22	1.96	0.46
1:H:218:ALA:HB2	1:H:232:VAL:HG22	1.97	0.46
1:B:264:ILE:HG22	1:B:265:ASN:H	1.80	0.46
1:H:38:VAL:HG11	1:H:80:TYR:CD2	2.50	0.46
1:H:50:PHE:HE1	1:H:73:ARG:HA	1.81	0.46
3:F:402[B]:NAP:O1A	3:F:402[B]:NAP:H52N	2.16	0.46
1:G:256:PHE:O	1:G:260:VAL:HG13	2.15	0.46
1:H:195:ILE:HG21	1:H:200:LEU:HD13	1.97	0.46
1:A:303:PHE:HB3	2:A:401:FAD:O2	2.16	0.46
1:B:267:ASN:O	1:B:269:PHE:N	2.49	0.46
1:F:109:ILE:HB	1:F:116:TYR:HB2	1.98	0.46
1:B:276:ASN:C	1:B:278:GLU:H	2.23	0.46
1:F:248:ILE:HA	3:F:402[B]:NAP:O4B	2.16	0.46
1:F:167:SER:HG	3:F:402[B]:NAP:PN	2.39	0.45
1:D:56:LYS:O	1:D:308:LYS:NZ	2.49	0.45
1:D:248:ILE:HA	3:D:402[B]:NAP:O4B	2.17	0.45
1:E:84:VAL:HG13	1:E:89:LEU:HB2	1.99	0.45
1:B:54:SER:O	1:B:64:PHE:HB3	2.16	0.45
1:G:275:TYR:HB3	1:G:282:THR:HG22	1.98	0.45
1:H:297:ASN:O	1:H:299:ALA:N	2.48	0.45
1:F:96:GLU:H	1:F:112:THR:HG1	1.61	0.45
1:G:48:GLN:NE2	1:G:170:ASP:OD2	2.41	0.45
1:B:11:GLY:N	1:B:33:GLU:OE1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:VAL:HG13	1:B:89:LEU:HB2	1.98	0.45
1:B:187:ARG:HG3	1:B:218:ALA:O	2.16	0.45
1:G:16:LEU:HD22	1:G:89:LEU:HD12	1.99	0.45
1:A:59:ILE:O	1:A:61:ASP:N	2.50	0.45
1:A:166:ASN:ND2	1:A:194:SER:O	2.49	0.45
1:G:21:GLU:O	1:G:25:LYS:HG2	2.17	0.45
1:D:260:VAL:HG22	1:D:262:ILE:HG13	1.99	0.45
1:F:182:VAL:HB	1:F:212:ILE:HG23	1.99	0.45
1:G:100:VAL:HB	1:G:260:VAL:HG12	1.98	0.44
1:D:167:SER:H	3:D:402[A]:NAP:H51N	1.83	0.44
1:E:104[B]:ASN:OD1	1:E:105:ASN:N	2.50	0.44
1:C:55:ASP:OD1	1:C:56:LYS:N	2.50	0.44
1:G:257:LEU:O	1:G:260:VAL:HG22	2.17	0.44
1:H:93:ALA:O	1:H:113:LYS:NZ	2.30	0.44
1:D:165:LYS:HD3	3:D:402[A]:NAP:O3D	2.17	0.44
1:B:107:PHE:O	1:B:117:GLU:HA	2.18	0.44
1:E:224:THR:HG1	1:E:227:THR:H	1.65	0.44
1:G:275:TYR:HA	1:G:282:THR:HA	1.99	0.44
1:G:291:GLY:H	1:G:310:HIS:CE1	2.36	0.44
1:C:73:ARG:O	1:C:76:ALA:N	2.49	0.44
1:G:97:VAL:HG22	1:G:111:THR:HG22	2.00	0.44
1:B:266:THR:HA	1:B:270:GLY:O	2.17	0.44
1:D:265:ASN:ND2	1:D:274:MET:HG3	2.33	0.44
1:G:258:LYS:HE3	1:G:264:ILE:HD12	1.98	0.44
1:H:201:PRO:HA	1:H:204:THR:HB	1.99	0.44
1:F:257:LEU:HD13	1:F:273:PRO:HG3	2.00	0.44
1:G:222:GLN:HB3	1:G:229:THR:HB	1.99	0.44
1:H:257:LEU:O	1:H:260:VAL:HG22	2.18	0.43
1:G:8:ILE:O	1:G:31:ILE:HA	2.18	0.43
1:A:169:ILE:HD13	1:A:169:ILE:HA	1.86	0.43
1:C:31:ILE:HB	1:C:91:VAL:HG22	2.01	0.43
1:G:17:SER:HA	1:G:20:ILE:HD12	2.00	0.43
1:C:99:THR:HG23	1:C:101:LYS:HE2	2.01	0.43
1:C:165:LYS:HE3	1:C:194:SER:OG	2.19	0.43
1:B:298:ASP:OD1	1:B:299:ALA:N	2.52	0.43
1:C:54:SER:OG	1:C:64:PHE:O	2.34	0.43
1:G:4:VAL:HG21	1:G:30:LEU:HD22	2.00	0.43
1:G:289:ILE:HD12	1:G:293:ILE:HG23	1.99	0.43
1:A:262:ILE:HD11	1:A:287:CYS:SG	2.58	0.43
1:H:304:ILE:N	1:H:308:LYS:HZ2	2.16	0.43
1:A:217:ASN:O	1:A:232:VAL:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:ASP:OD1	1:E:226:ASP:N	2.50	0.43
1:A:13:PRO:HD3	1:A:38:VAL:HG12	2.00	0.43
1:F:165:LYS:HD3	3:F:402[A]:NAP:O3D	2.18	0.43
1:G:161:ILE:HD11	1:G:175:LEU:HD12	1.99	0.43
1:H:63:PRO:HG2	1:H:64:PHE:CE2	2.54	0.43
2:H:401:FAD:H9	2:H:401:FAD:H1'1	1.85	0.43
1:G:127:TYR:CE2	1:G:292:VAL:HB	2.54	0.42
1:C:128[A]:TYR:CZ	2:C:401:FAD:H9	2.54	0.42
1:B:67:GLU:HA	1:C:78:VAL:HG21	2.01	0.42
1:C:150:GLU:CD	1:D:73:ARG:HH22	2.24	0.42
1:E:286:ASN:OD1	1:E:321:LYS:NZ	2.38	0.42
1:H:56:LYS:CB	1:H:306:ASN:HB2	2.48	0.42
1:F:165:LYS:NZ	3:F:402[B]:NAP:O1X	2.49	0.42
1:C:257:LEU:HD11	1:C:293:ILE:HD11	2.00	0.42
1:H:23:LYS:NZ	1:H:88:GLN:O	2.52	0.42
1:D:226:ASP:OD1	1:D:226:ASP:N	2.52	0.42
1:E:101:LYS:HA	1:E:101:LYS:HD3	1.92	0.42
1:G:226:ASP:OD1	1:G:226:ASP:N	2.53	0.42
1:C:25:LYS:HG3	1:C:315:ALA:HB1	2.02	0.42
1:F:6:SER:HB3	1:F:29:THR:HG22	2.02	0.42
1:H:160:VAL:HB	1:H:244:VAL:HG22	2.02	0.42
1:A:149:LYS:HD2	1:A:149:LYS:HA	1.95	0.42
1:D:6:SER:HB3	1:D:29:THR:HG22	2.00	0.42
1:D:165:LYS:HB3	3:D:402[A]:NAP:O3D	2.20	0.42
1:F:262:ILE:HD13	1:F:282:THR:HG21	2.01	0.42
1:A:8:ILE:HG12	1:A:122:THR:HB	2.02	0.41
1:F:120:PHE:CG	1:F:318:MET:HE3	2.54	0.41
1:G:257:LEU:HD23	1:G:257:LEU:HA	1.93	0.41
1:H:166:ASN:ND2	1:H:194:SER:O	2.52	0.41
1:E:120:PHE:CD2	1:E:318:MET:HE3	2.54	0.41
1:F:288:TYR:CD2	1:F:314:ILE:HG23	2.55	0.41
1:G:49:THR:OG1	1:G:72:ARG:HG2	2.19	0.41
1:G:173:LEU:O	1:G:177:LYS:HG2	2.19	0.41
1:G:262:ILE:HG21	1:G:273:PRO:HB3	2.02	0.41
1:H:11:GLY:N	1:H:33:GLU:OE1	2.34	0.41
1:H:126:GLY:HA2	1:H:292:VAL:HG23	2.01	0.41
1:A:226:ASP:OD1	1:A:226:ASP:N	2.53	0.41
1:F:128:TYR:OH	2:F:401:FAD:H9	2.20	0.41
1:F:187:ARG:HH21	3:F:402[A]:NAP:P2B	2.43	0.41
1:F:226:ASP:N	1:F:226:ASP:OD1	2.53	0.41
1:D:131:HIS:HA	1:D:250:TYR:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:304:ILE:H	1:H:308:LYS:HZ2	1.67	0.41
1:A:65:ILE:CG1	1:D:82:GLU:HG3	2.47	0.41
1:B:35:GLY:HA3	1:B:39:GLU:HG3	2.03	0.41
1:G:275:TYR:CE2	1:G:289:ILE:HD11	2.55	0.41
1:E:9:ILE:HD13	1:E:97:VAL:HG11	2.03	0.41
1:F:2:GLN:HG3	1:F:114:ASP:OD2	2.20	0.41
1:H:95:GLU:HB2	1:H:113:LYS:HD2	2.01	0.41
1:A:2:GLN:HG3	1:A:114:ASP:OD2	2.21	0.41
1:D:31:ILE:HB	1:D:91:VAL:HG22	2.01	0.41
1:B:82:GLU:HG3	1:C:65:ILE:HG12	2.03	0.41
1:D:33:GLU:HG3	1:D:35:GLY:C	2.46	0.41
1:B:78:VAL:HG21	1:C:67:GLU:HA	2.03	0.40
1:C:63:PRO:HB2	1:C:65:ILE:HD12	2.03	0.40
1:E:132:ASN:HB2	1:E:248:ILE:HG13	2.03	0.40
1:F:62:VAL:O	1:F:79:TYR:OH	2.36	0.40
1:G:262:ILE:HD13	1:G:282:THR:HG21	2.02	0.40
1:H:158:ASP:HB3	1:H:241:ASN:HA	2.01	0.40
1:H:164:GLY:HA3	1:H:186:TYR:CE2	2.56	0.40
1:C:39:GLU:OE2	1:C:43:ASN:ND2	2.55	0.40
1:D:165:LYS:HE3	1:D:194:SER:OG	2.22	0.40
1:E:316:GLN:O	1:E:320:ALA:N	2.54	0.40
1:H:73:ARG:H	1:H:73:ARG:HG3	1.48	0.40
1:H:158:ASP:HA	1:H:181:ASN:HB2	2.03	0.40
1:E:260:VAL:HG22	1:E:262:ILE:HG13	2.03	0.40
1:G:106:LYS:NZ	1:G:119:ARG:HG2	2.35	0.40
1:H:288:TYR:CD2	1:H:314:ILE:HG23	2.56	0.40
1:A:198:TRP:CD1	1:A:199:ILE:HG13	2.57	0.40
1:A:267:ASN:O	1:F:271:THR:HG21	2.21	0.40
1:C:167:SER:HA	3:C:402:NAP:H5N	2.03	0.40
1:F:128:TYR:OH	2:F:401:FAD:H1'1	2.22	0.40
1:F:297:ASN:O	1:F:299:ALA:N	2.55	0.40
1:G:97:VAL:HA	1:G:111:THR:HG22	2.03	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	324/328 (99%)	301 (93%)	21 (6%)	2 (1%)	22	53
1	B	321/328 (98%)	305 (95%)	15 (5%)	1 (0%)	37	68
1	C	325/328 (99%)	302 (93%)	17 (5%)	6 (2%)	7	29
1	D	323/328 (98%)	304 (94%)	15 (5%)	4 (1%)	11	38
1	E	323/328 (98%)	297 (92%)	21 (6%)	5 (2%)	8	33
1	F	324/328 (99%)	303 (94%)	16 (5%)	5 (2%)	8	33
1	G	287/328 (88%)	254 (88%)	27 (9%)	6 (2%)	5	25
1	H	316/328 (96%)	275 (87%)	25 (8%)	16 (5%)	1	10
All	All	2543/2624 (97%)	2341 (92%)	157 (6%)	45 (2%)	7	29

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLY
1	A	298	ASP
1	C	73	ARG
1	C	271	THR
1	E	73	ARG
1	E	299	ALA
1	F	298	ASP
1	H	165	LYS
1	H	166	ASN
1	H	297	ASN
1	H	312	GLY
1	C	74	ASN
1	C	296	GLY
1	E	60	GLY
1	E	74	ASN
1	F	60	GLY
1	G	92	ASN
1	G	265	ASN
1	G	296	GLY
1	H	72	ARG
1	H	164	GLY
1	H	264	ILE
1	H	304	ILE

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Mol	Chain	Res	Type
1	D	266	THR
1	D	298	ASP
1	F	299	ALA
1	G	93	ALA
1	H	299	ALA
1	C	94	PHE
1	C	298	ASP
1	D	94	PHE
1	D	267	ASN
1	F	94	PHE
1	H	50	PHE
1	H	63	PRO
1	H	277	LYS
1	B	268	GLU
1	E	94	PHE
1	F	267	ASN
1	G	63	PRO
1	G	270	GLY
1	H	61	ASP
1	H	64	PHE
1	H	309	PHE
1	H	66	VAL

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	280/282 (99%)	270 (96%)	10 (4%)	30	60
1	B	277/282 (98%)	273 (99%)	4 (1%)	62	81
1	C	281/282 (100%)	274 (98%)	7 (2%)	42	69
1	D	279/282 (99%)	269 (96%)	10 (4%)	30	60
1	E	279/282 (99%)	264 (95%)	15 (5%)	18	47
1	F	280/282 (99%)	269 (96%)	11 (4%)	27	58
1	G	250/282 (89%)	240 (96%)	10 (4%)	27	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	273/282 (97%)	265 (97%)	8 (3%)	37 65
All	All	2199/2256 (98%)	2124 (97%)	75 (3%)	32 62

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	65	ILE
1	A	68	GLU
1	A	99	THR
1	A	104	ASN
1	A	112	THR
1	A	136	VAL
1	A	232	VAL
1	A	268	GLU
1	A	322	LYS
1	B	69	SER
1	B	156	ASP
1	B	160	VAL
1	B	305	GLU
1	C	39	GLU
1	C	65	ILE
1	C	112	THR
1	C	136	VAL
1	C	209	HIS
1	C	303	PHE
1	C	322	LYS
1	D	39	GLU
1	D	46	THR
1	D	99	THR
1	D	136	VAL
1	D	207	VAL
1	D	260	VAL
1	D	271	THR
1	D	297	ASN
1	D	301	THR
1	D	303	PHE
1	E	39	GLU
1	E	65	ILE
1	E	99	THR
1	E	103	MET
1	E	112	THR

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Mol	Chain	Res	Type
1	E	136	VAL
1	E	204	THR
1	E	260	VAL
1	E	266	THR
1	E	268	GLU
1	E	274	MET
1	E	275	TYR
1	E	301	THR
1	E	303	PHE
1	E	322	LYS
1	F	46	THR
1	F	55	ASP
1	F	65	ILE
1	F	91	VAL
1	F	102	LYS
1	F	112	THR
1	F	136	VAL
1	F	199	ILE
1	F	260	VAL
1	F	293	ILE
1	F	303	PHE
1	G	46	THR
1	G	68	GLU
1	G	69	SER
1	G	85	LYS
1	G	95	GLU
1	G	99	THR
1	G	136	VAL
1	G	242	ASP
1	G	260	VAL
1	G	303	PHE
1	H	47	HIS
1	H	156	ASP
1	H	160	VAL
1	H	186	TYR
1	H	204	THR
1	H	260	VAL
1	H	303	PHE
1	H	310	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	86	HIS
1	A	208	ASN
1	B	157	GLN
1	B	208	ASN
1	B	217	ASN
1	B	222	GLN
1	B	265	ASN
1	B	297	ASN
1	C	48	GLN
1	C	86	HIS
1	C	157	GLN
1	C	219	ASN
1	D	2	GLN
1	D	104	ASN
1	D	130	GLN
1	D	166	ASN
1	D	202	ASN
1	D	219	ASN
1	D	265	ASN
1	E	48	GLN
1	E	88	GLN
1	F	86	HIS
1	F	104	ASN
1	F	146	HIS
1	F	157	GLN
1	F	217	ASN
1	F	265	ASN
1	F	297	ASN
1	G	86	HIS
1	G	217	ASN
1	H	43	ASN
1	H	75	GLN
1	H	233	ASN
1	H	306	ASN
1	H	310	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
3	NAP	F	402[B]	-	45,52,52	0.70	1 (2%)	56,80,80	0.98	3 (5%)
2	FAD	C	401	-	53,58,58	0.46	0	68,89,89	0.53	1 (1%)
3	NAP	C	402	-	45,52,52	0.68	1 (2%)	56,80,80	0.79	3 (5%)
3	NAP	D	402[B]	-	45,52,52	0.67	1 (2%)	56,80,80	0.88	3 (5%)
3	NAP	D	402[A]	-	45,52,52	0.67	1 (2%)	56,80,80	0.80	3 (5%)
2	FAD	E	401	-	53,58,58	0.47	0	68,89,89	0.52	1 (1%)
2	FAD	A	401	-	53,58,58	0.46	0	68,89,89	0.57	2 (2%)
3	NAP	F	402[A]	-	45,52,52	0.69	1 (2%)	56,80,80	0.74	2 (3%)
2	FAD	D	401	-	53,58,58	0.47	0	68,89,89	0.55	1 (1%)
2	FAD	F	401	-	53,58,58	0.47	0	68,89,89	0.54	1 (1%)
2	FAD	H	401	-	53,58,58	0.45	0	68,89,89	0.57	2 (2%)
2	FAD	G	401	-	53,58,58	0.46	0	68,89,89	0.50	2 (2%)
2	FAD	B	401	-	53,58,58	0.46	0	68,89,89	0.54	2 (2%)

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
3	NAP	F	402[B]	-	-	10/31/67/67	0/5/5/5
2	FAD	C	401	-	-	3/30/50/50	0/6/6/6
3	NAP	C	402	-	-	7/31/67/67	0/5/5/5
3	NAP	D	402[B]	-	-	17/31/67/67	0/5/5/5
3	NAP	D	402[A]	-	-	6/31/67/67	0/5/5/5
2	FAD	E	401	-	-	3/30/50/50	0/6/6/6
2	FAD	A	401	-	-	3/30/50/50	0/6/6/6
3	NAP	F	402[A]	-	-	6/31/67/67	0/5/5/5
2	FAD	D	401	-	-	3/30/50/50	0/6/6/6
2	FAD	F	401	-	-	4/30/50/50	0/6/6/6
2	FAD	H	401	-	-	9/30/50/50	0/6/6/6
2	FAD	G	401	-	-	16/30/50/50	0/6/6/6
2	FAD	B	401	-	-	2/30/50/50	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402[B]	NAP	C2N-N1N	2.55	1.38	1.35
3	F	402[A]	NAP	C2N-N1N	2.18	1.37	1.35
3	D	402[A]	NAP	C2N-N1N	2.12	1.37	1.35
3	C	402	NAP	C2N-N1N	2.07	1.37	1.35
3	D	402[B]	NAP	C2N-N1N	2.06	1.37	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402[B]	NAP	O4D-C1D-C2D	-5.04	99.56	106.93
3	D	402[B]	NAP	O4D-C1D-C2D	-3.61	101.65	106.93
3	C	402	NAP	C6N-N1N-C2N	-2.58	119.62	121.97
3	D	402[A]	NAP	C6N-N1N-C2N	-2.52	119.68	121.97
2	H	401	FAD	P-O3P-PA	-2.49	124.28	132.83
3	F	402[B]	NAP	C6N-N1N-C2N	-2.45	119.75	121.97
2	A	401	FAD	P-O3P-PA	-2.44	124.44	132.83
3	D	402[A]	NAP	C5A-C6A-N6A	2.43	124.04	120.35
3	D	402[A]	NAP	C3D-C2D-C1D	2.37	104.55	100.98
3	C	402	NAP	O4D-C1D-C2D	-2.37	103.47	106.93
2	B	401	FAD	C5A-C6A-N6A	2.34	123.91	120.35
2	C	401	FAD	C5A-C6A-N6A	2.33	123.90	120.35
2	D	401	FAD	C5A-C6A-N6A	2.33	123.89	120.35
3	F	402[A]	NAP	C5A-C6A-N6A	2.33	123.89	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	FAD	C5A-C6A-N6A	2.30	123.85	120.35
2	A	401	FAD	C5A-C6A-N6A	2.29	123.83	120.35
2	F	401	FAD	C5A-C6A-N6A	2.28	123.82	120.35
2	G	401	FAD	P-O3P-PA	-2.27	125.03	132.83
2	B	401	FAD	P-O3P-PA	-2.27	125.03	132.83
2	H	401	FAD	C5A-C6A-N6A	2.26	123.79	120.35
2	E	401	FAD	C5A-C6A-N6A	2.26	123.79	120.35
3	F	402[B]	NAP	C5A-C6A-N6A	2.26	123.79	120.35
3	C	402	NAP	C5A-C6A-N6A	2.26	123.78	120.35
3	F	402[A]	NAP	C6N-N1N-C2N	-2.20	119.97	121.97
3	D	402[B]	NAP	C5A-C6A-N6A	2.16	123.64	120.35
3	D	402[B]	NAP	C6N-N1N-C2N	-2.07	120.09	121.97

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	401	FAD	C5B-O5B-PA-O1A
2	G	401	FAD	C5B-O5B-PA-O2A
2	G	401	FAD	C3B-C4B-C5B-O5B
2	G	401	FAD	C2'-C3'-C4'-O4'
2	G	401	FAD	C2'-C3'-C4'-C5'
2	G	401	FAD	O3'-C3'-C4'-O4'
2	G	401	FAD	O3'-C3'-C4'-C5'
2	G	401	FAD	C5'-O5'-P-O2P
2	H	401	FAD	N10-C1'-C2'-O2'
2	H	401	FAD	C2'-C3'-C4'-O4'
2	H	401	FAD	C2'-C3'-C4'-C5'
2	H	401	FAD	O3'-C3'-C4'-O4'
2	H	401	FAD	O3'-C3'-C4'-C5'
2	H	401	FAD	C3'-C4'-C5'-O5'
2	H	401	FAD	O4'-C4'-C5'-O5'
3	C	402	NAP	C2N-C3N-C7N-O7N
3	C	402	NAP	C2N-C3N-C7N-N7N
3	D	402[A]	NAP	O4D-C4D-C5D-O5D
3	D	402[B]	NAP	C5B-O5B-PA-O2A
3	D	402[B]	NAP	C5D-O5D-PN-O3
3	D	402[B]	NAP	O4D-C4D-C5D-O5D
3	D	402[B]	NAP	C3D-C4D-C5D-O5D
3	D	402[B]	NAP	C2N-C3N-C7N-O7N
3	D	402[B]	NAP	C2N-C3N-C7N-N7N
3	F	402[A]	NAP	C3B-C2B-O2B-P2B

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Mol	Chain	Res	Type	Atoms
3	F	402[B]	NAP	O4D-C4D-C5D-O5D
3	F	402[B]	NAP	C3D-C4D-C5D-O5D
3	C	402	NAP	C4N-C3N-C7N-N7N
3	C	402	NAP	C4N-C3N-C7N-O7N
3	D	402[B]	NAP	C4N-C3N-C7N-O7N
3	D	402[B]	NAP	C4N-C3N-C7N-N7N
2	A	401	FAD	O4B-C4B-C5B-O5B
2	A	401	FAD	C3B-C4B-C5B-O5B
2	G	401	FAD	O4B-C4B-C5B-O5B
3	D	402[A]	NAP	C3D-C4D-C5D-O5D
3	D	402[B]	NAP	O4B-C4B-C5B-O5B
3	D	402[B]	NAP	C3B-C4B-C5B-O5B
3	F	402[A]	NAP	O4D-C4D-C5D-O5D
3	F	402[A]	NAP	C3D-C4D-C5D-O5D
3	F	402[B]	NAP	C2N-C3N-C7N-O7N
3	F	402[B]	NAP	C2N-C3N-C7N-N7N
3	D	402[A]	NAP	C3B-C2B-O2B-P2B
3	F	402[B]	NAP	C4N-C3N-C7N-N7N
3	D	402[B]	NAP	C1B-C2B-O2B-P2B
3	C	402	NAP	C3B-C2B-O2B-P2B
3	D	402[B]	NAP	C3B-C2B-O2B-P2B
3	F	402[B]	NAP	C3B-C2B-O2B-P2B
3	F	402[B]	NAP	C4N-C3N-C7N-O7N
3	C	402	NAP	C1B-C2B-O2B-P2B
3	D	402[A]	NAP	C1B-C2B-O2B-P2B
3	F	402[A]	NAP	C1B-C2B-O2B-P2B
3	F	402[B]	NAP	C1B-C2B-O2B-P2B
3	D	402[A]	NAP	C4D-C5D-O5D-PN
3	D	402[B]	NAP	PA-O3-PN-O1N
3	F	402[A]	NAP	C4D-C5D-O5D-PN
2	H	401	FAD	C4'-C5'-O5'-P
2	A	401	FAD	PA-O3P-P-O5'
2	B	401	FAD	PA-O3P-P-O5'
2	C	401	FAD	PA-O3P-P-O5'
2	D	401	FAD	PA-O3P-P-O5'
2	E	401	FAD	PA-O3P-P-O5'
2	F	401	FAD	PA-O3P-P-O5'
2	G	401	FAD	PA-O3P-P-O5'
2	G	401	FAD	C5'-O5'-P-O3P
3	D	402[B]	NAP	C5B-O5B-PA-O3
2	G	401	FAD	C5'-O5'-P-O1P
3	D	402[B]	NAP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	D	402[B]	NAP	PA-O3-PN-O2N
3	F	402[B]	NAP	O4B-C4B-C5B-O5B
3	F	402[B]	NAP	C4D-C5D-O5D-PN
2	E	401	FAD	P-O3P-PA-O2A
2	G	401	FAD	C5B-O5B-PA-O3P
2	B	401	FAD	O4B-C4B-C5B-O5B
2	C	401	FAD	O4B-C4B-C5B-O5B
2	E	401	FAD	O4B-C4B-C5B-O5B
3	C	402	NAP	O4B-C4B-C5B-O5B
3	D	402[A]	NAP	O4B-C4B-C5B-O5B
2	C	401	FAD	P-O3P-PA-O2A
2	D	401	FAD	P-O3P-PA-O2A
2	F	401	FAD	P-O3P-PA-O1A
2	F	401	FAD	P-O3P-PA-O2A
2	H	401	FAD	C5B-O5B-PA-O1A
3	D	402[B]	NAP	C5D-O5D-PN-O1N
2	D	401	FAD	O4B-C4B-C5B-O5B
2	F	401	FAD	O4B-C4B-C5B-O5B
3	F	402[A]	NAP	O4B-C4B-C5B-O5B
2	G	401	FAD	C1'-C2'-C3'-O3'
2	G	401	FAD	O2'-C2'-C3'-O3'
2	G	401	FAD	N10-C1'-C2'-O2'

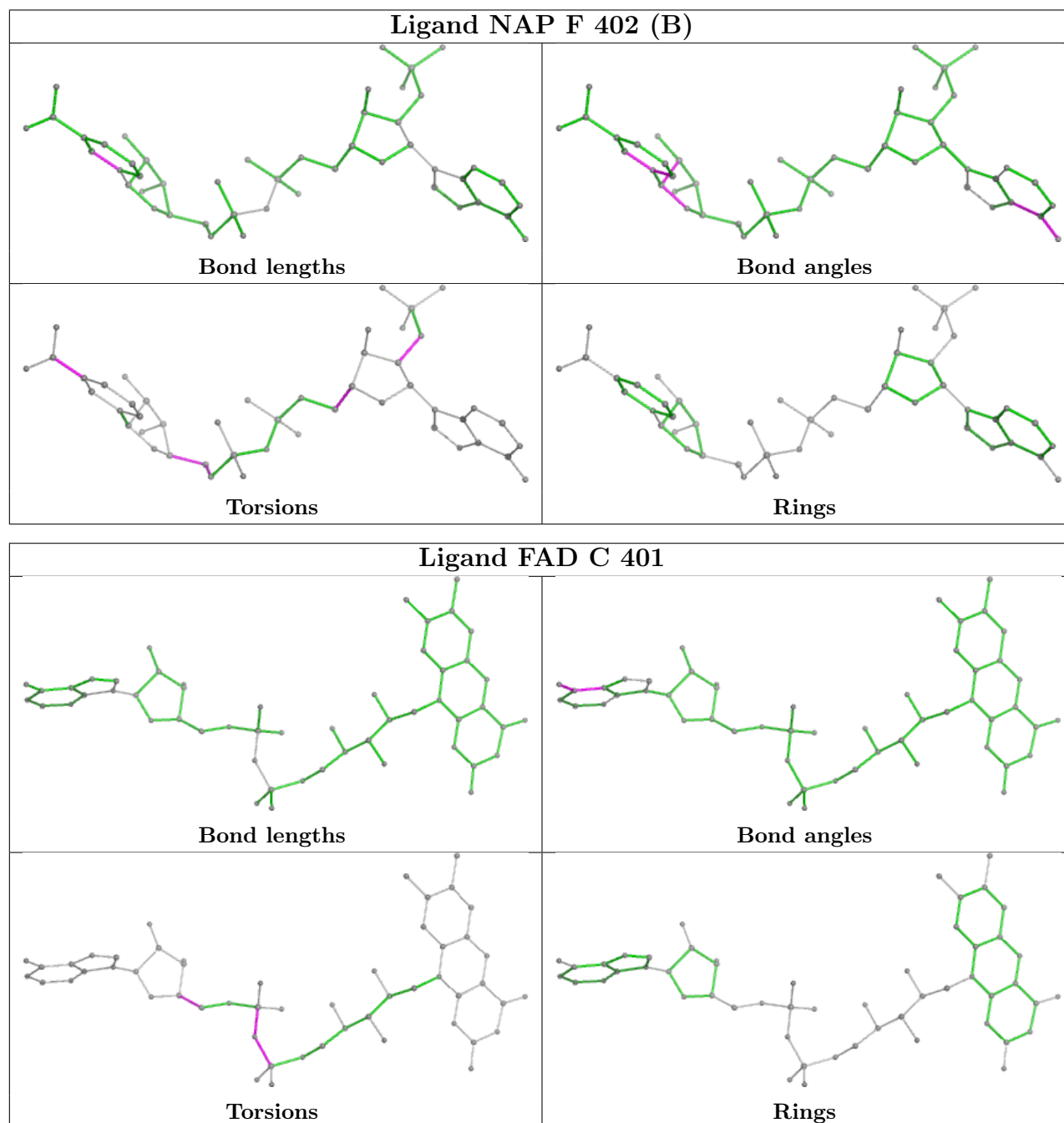
There are no ring outliers.

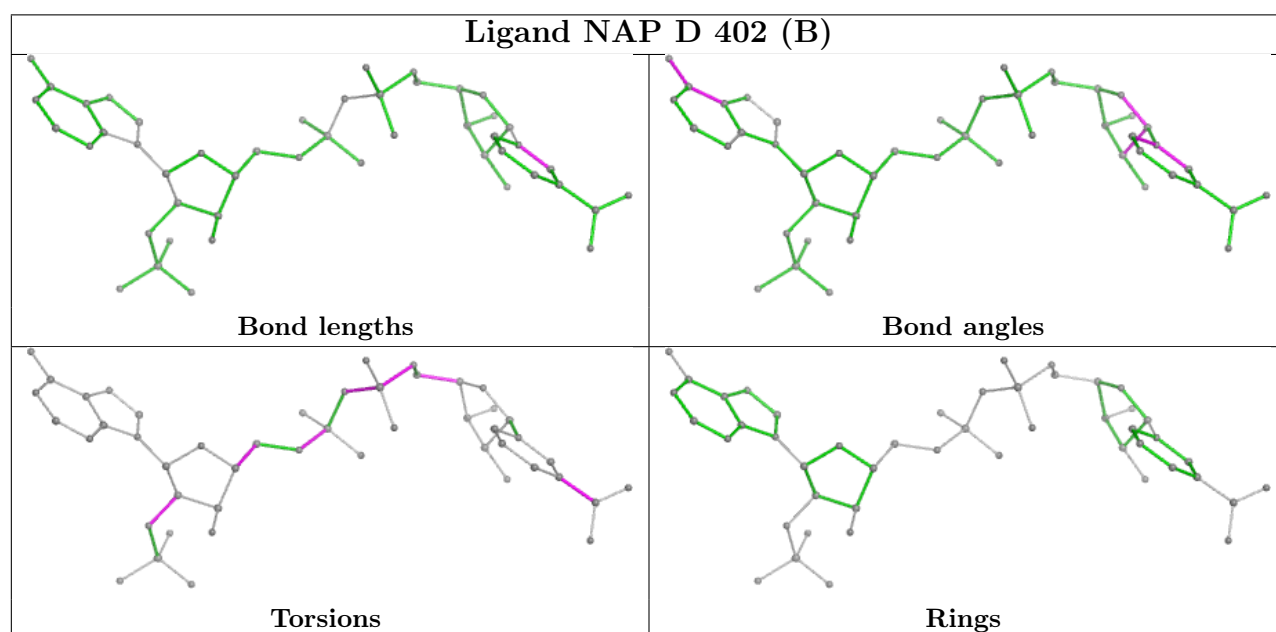
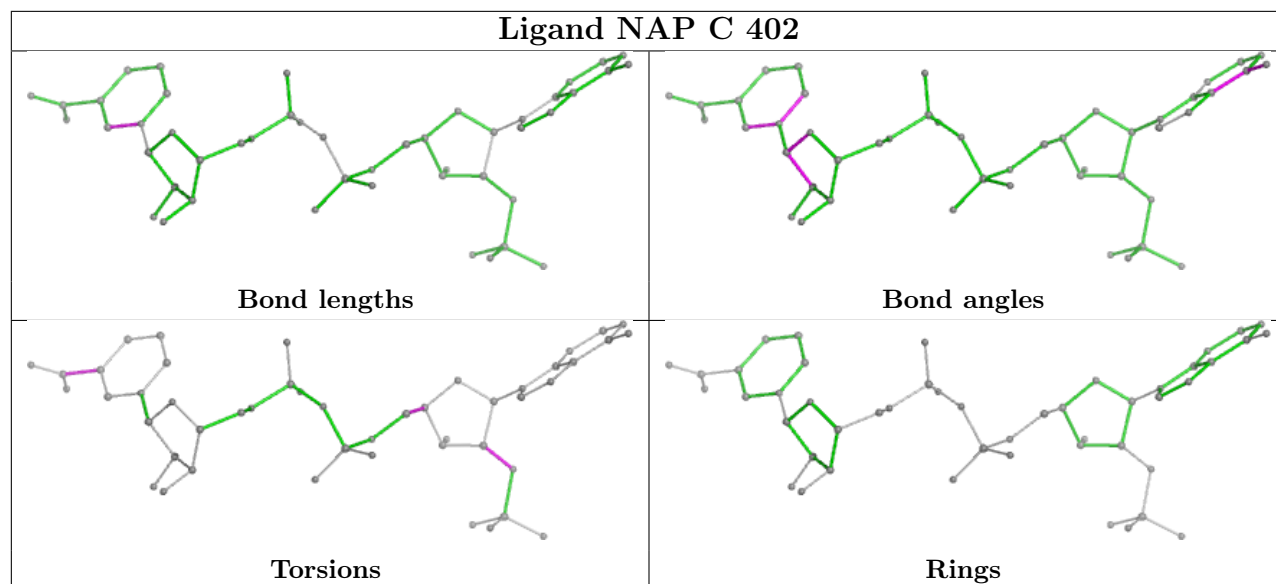
10 monomers are involved in 25 short contacts:

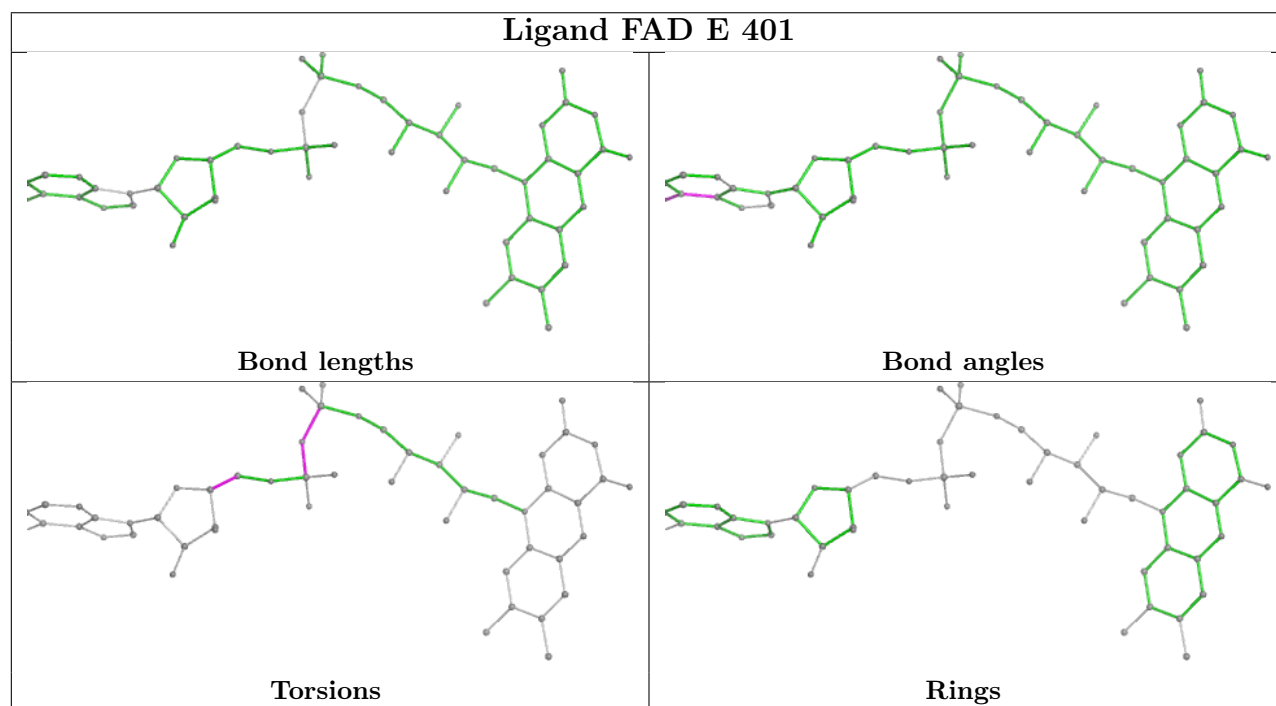
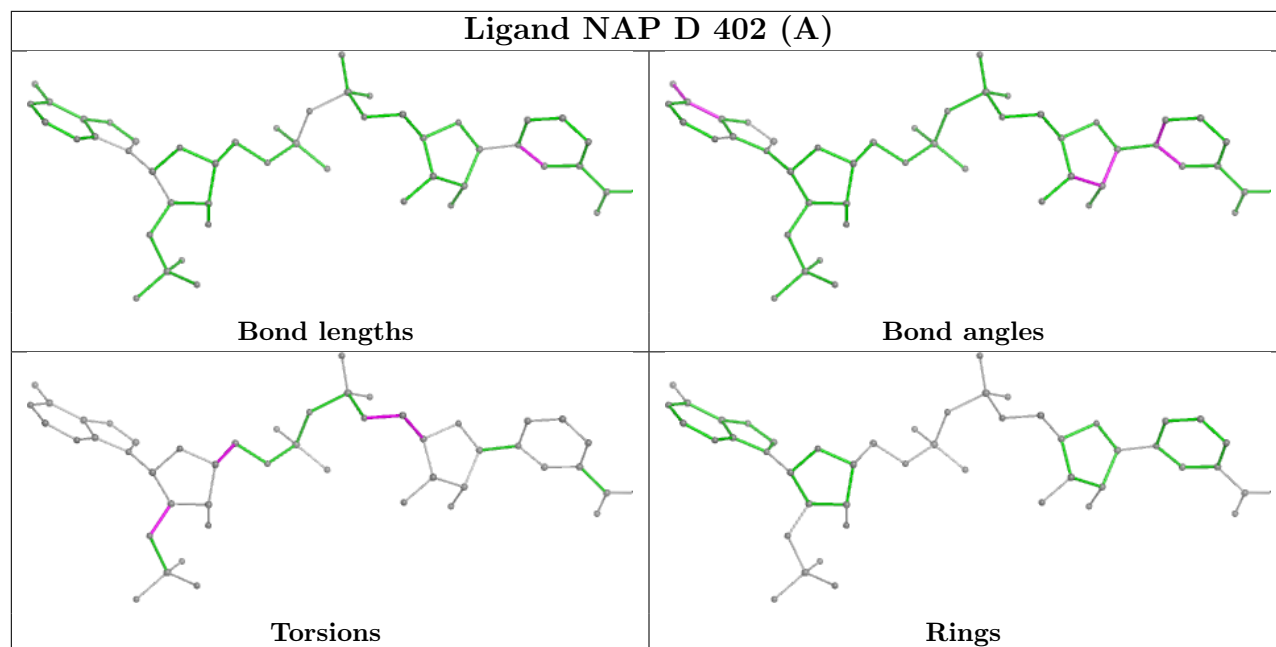
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	402[B]	NAP	5	0
2	C	401	FAD	3	0
3	C	402	NAP	1	0
3	D	402[B]	NAP	2	0
3	D	402[A]	NAP	4	0
2	A	401	FAD	1	0
3	F	402[A]	NAP	3	0
2	D	401	FAD	1	0
2	F	401	FAD	2	0
2	H	401	FAD	3	0

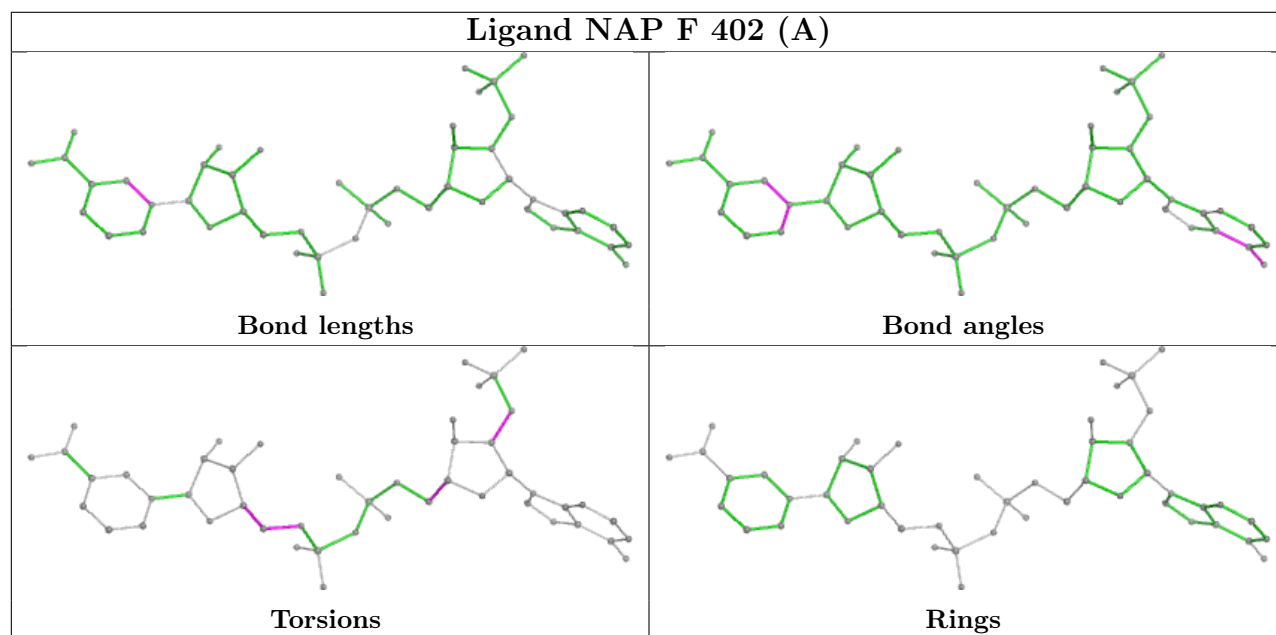
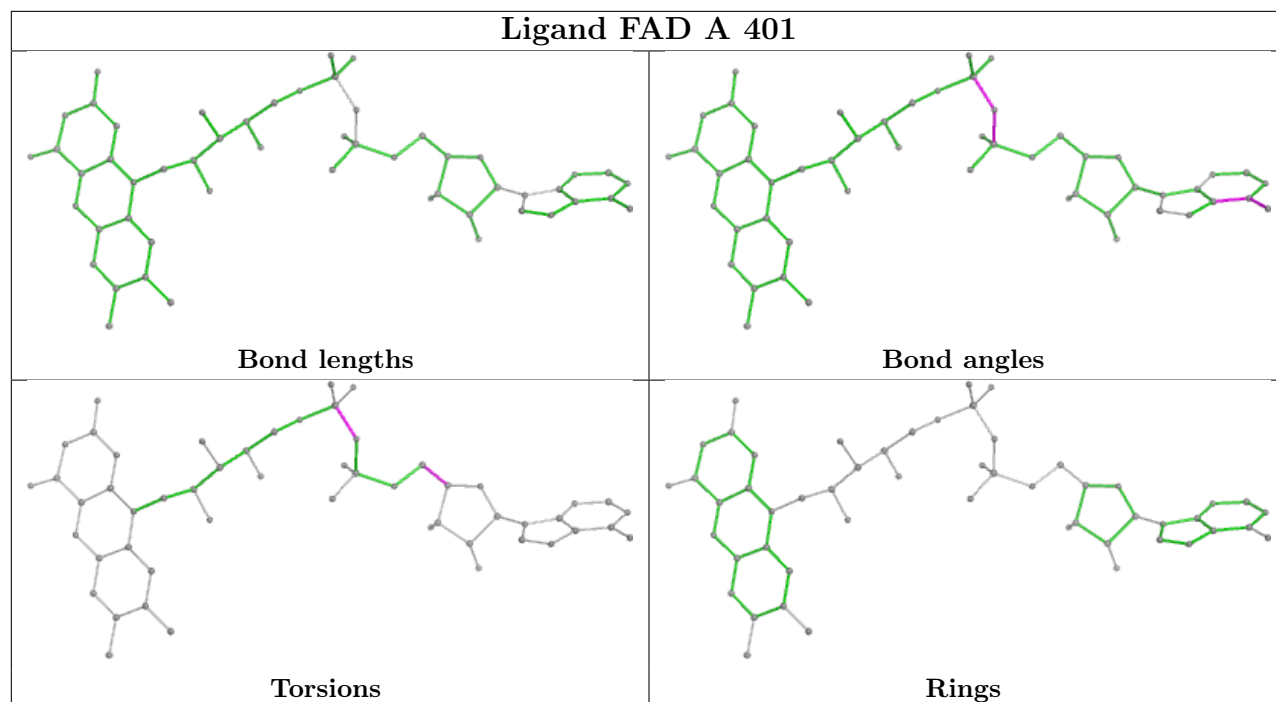
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

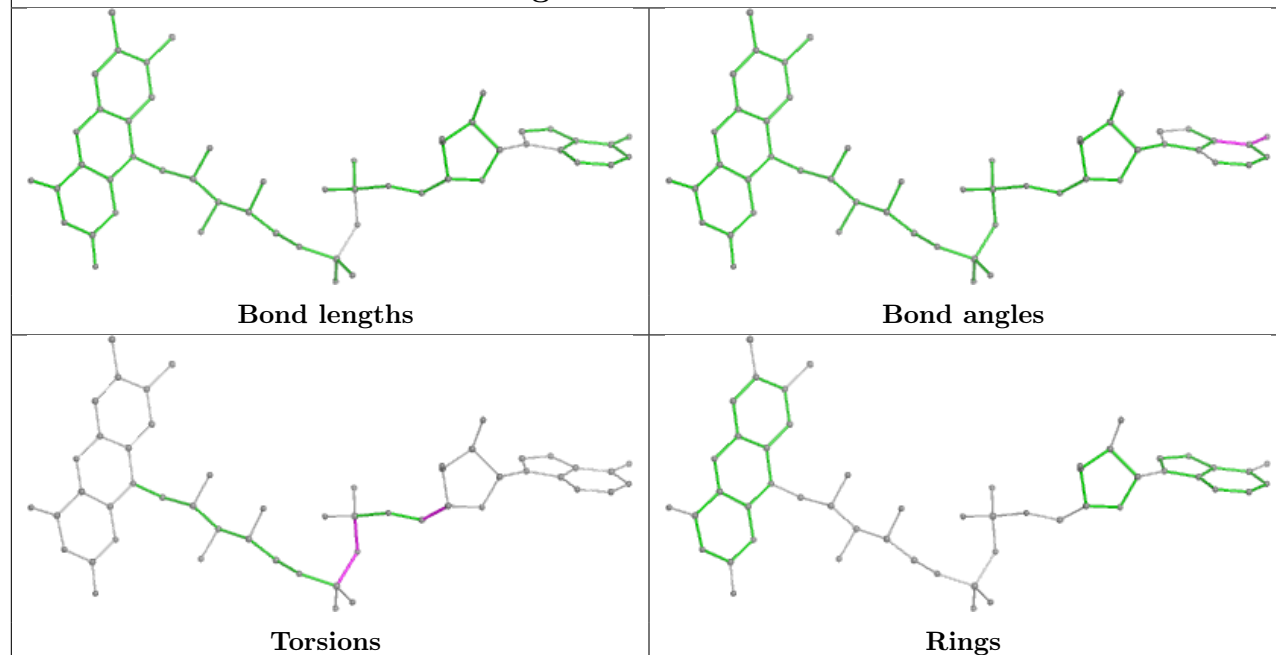




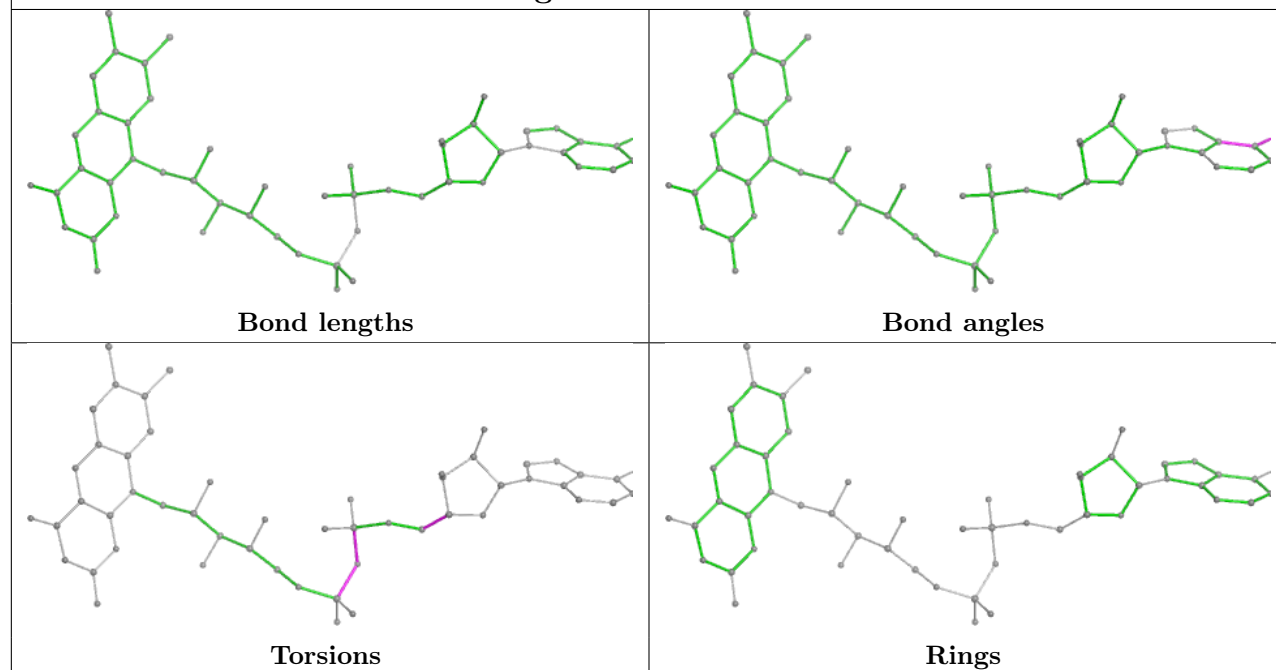


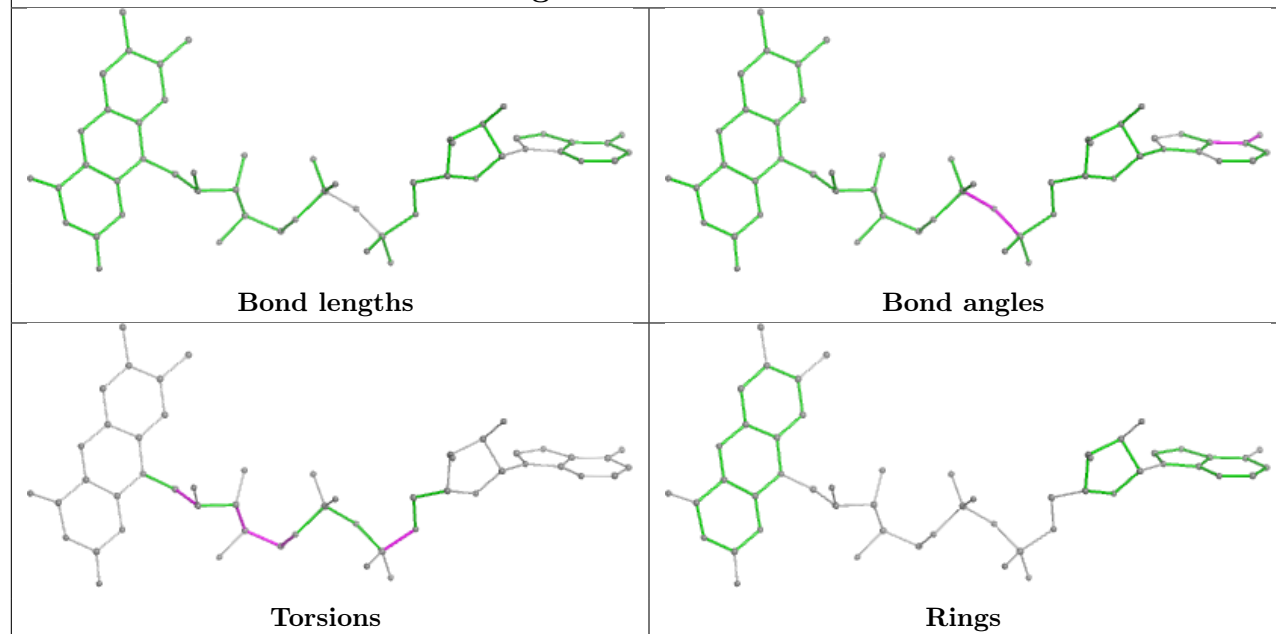
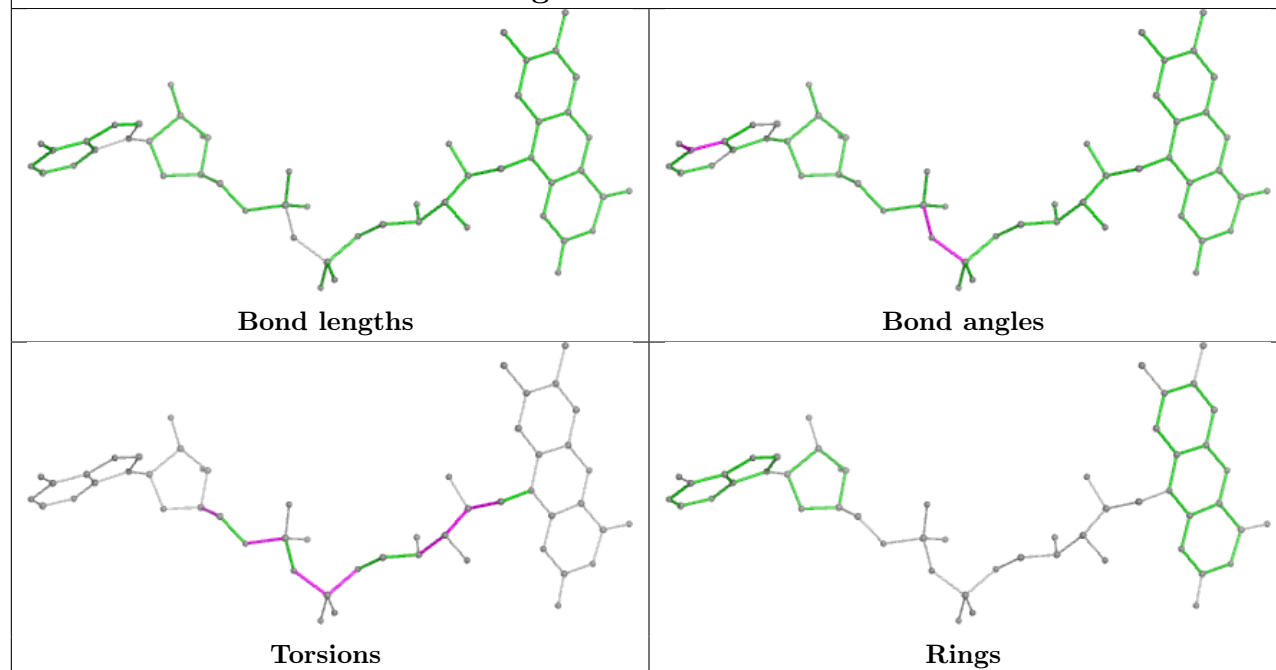


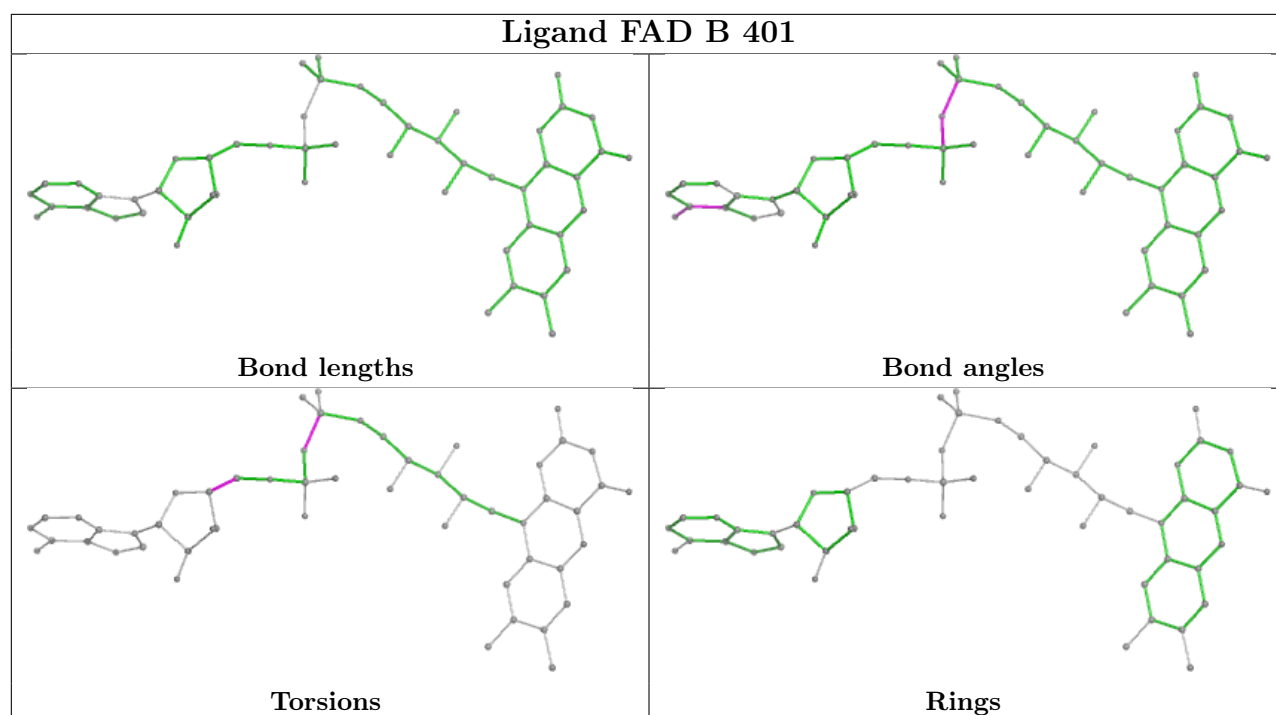
Ligand FAD D 401



Ligand FAD F 401



Ligand FAD H 401**Ligand FAD G 401**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/328 (98%)	-0.09	5 (1%) 71 54	18, 55, 87, 117	3 (0%)
1	B	322/328 (98%)	-0.19	4 (1%) 76 60	21, 55, 98, 130	1 (0%)
1	C	323/328 (98%)	-0.34	2 (0%) 85 72	19, 44, 73, 108	4 (1%)
1	D	323/328 (98%)	-0.32	0 100 100	18, 46, 80, 114	2 (0%)
1	E	323/328 (98%)	-0.35	3 (0%) 81 66	19, 44, 79, 116	2 (0%)
1	F	323/328 (98%)	-0.22	3 (0%) 81 66	23, 48, 88, 112	3 (0%)
1	G	293/328 (89%)	1.51	91 (31%) 1 1	70, 122, 148, 169	0
1	H	318/328 (96%)	1.60	99 (31%) 1 1	77, 118, 163, 176	0
All	All	2548/2624 (97%)	0.18	207 (8%) 19 11	18, 55, 138, 176	15 (0%)

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	91	VAL	7.6
1	G	63	PRO	6.3
1	H	42	TYR	5.9
1	H	63	PRO	5.3
1	H	175	LEU	5.2
1	H	151	ALA	5.2
1	H	178	ALA	4.7
1	G	71	PRO	4.6
1	H	71	PRO	4.5
1	G	64	PHE	4.4
1	G	11	GLY	4.3
1	C	128[A]	TYR	4.1
1	G	95	GLU	4.1
1	H	180	ALA	4.1
1	H	233	ASN	4.1
1	H	186	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	274	MET	3.9
1	H	216	PHE	3.9
1	G	195	ILE	3.8
1	G	148	PHE	3.8
1	H	66	VAL	3.7
1	H	182	VAL	3.6
1	H	289	ILE	3.6
1	H	291	GLY	3.5
1	H	77	LEU	3.5
1	G	177	LYS	3.5
1	G	32	ILE	3.4
1	G	290	ALA	3.4
1	G	289	ILE	3.4
1	G	178	ALA	3.3
1	H	179	GLY	3.3
1	H	234	GLY	3.3
1	H	217	ASN	3.3
1	H	302	ILE	3.3
1	H	275	TYR	3.3
1	H	38	VAL	3.3
1	H	16	LEU	3.3
1	H	128	TYR	3.3
1	H	160	VAL	3.3
1	G	313	ILE	3.3
1	G	269	PHE	3.2
1	G	273	PRO	3.2
1	H	174	GLU	3.2
1	H	185	LEU	3.2
1	G	62	VAL	3.2
1	G	280	TYR	3.1
1	E	300	ASN	3.1
1	G	100	VAL	3.1
1	G	51	PHE	3.1
1	G	134	LEU	3.1
1	H	218	ALA	3.1
1	G	305	GLU	3.1
1	F	299	ALA	3.1
1	G	150	GLU	3.0
1	G	309	PHE	3.0
1	G	8	ILE	3.0
1	H	158	ASP	3.0
1	G	112	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	64	PHE	3.0
1	H	299	ALA	3.0
1	G	96	GLU	2.9
1	G	114	ASP	2.9
1	B	47[A]	HIS	2.9
1	C	47[A]	HIS	2.9
1	G	266	THR	2.9
1	G	113	LYS	2.9
1	G	109	ILE	2.9
1	H	300	ASN	2.8
1	G	176	GLU	2.8
1	H	290	ALA	2.8
1	H	41	ILE	2.8
1	G	37	VAL	2.8
1	G	84	VAL	2.8
1	G	293	ILE	2.8
1	H	264	ILE	2.8
1	H	45	PRO	2.7
1	A	298	ASP	2.7
1	G	147	TYR	2.7
1	G	16	LEU	2.7
1	G	115	VAL	2.7
1	H	161	ILE	2.7
1	G	13	PRO	2.7
1	H	303	PHE	2.7
1	H	304	ILE	2.7
1	G	70	LYS	2.7
1	G	257	LEU	2.7
1	G	303	PHE	2.7
1	H	148	PHE	2.7
1	H	183	THR	2.7
1	H	273	PRO	2.7
1	H	184	VAL	2.7
1	A	300	ASN	2.7
1	H	26	GLY	2.7
1	H	311	GLY	2.7
1	G	175	LEU	2.7
1	G	277	LYS	2.6
1	H	46	THR	2.6
1	G	169	ILE	2.6
1	G	151	ALA	2.6
1	H	121	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	206	LEU	2.6
1	B	300	ASN	2.6
1	G	99	THR	2.6
1	G	302	ILE	2.6
1	H	262	ILE	2.6
1	G	1	MET	2.6
1	G	52	SER	2.6
1	H	209	HIS	2.6
1	G	89	LEU	2.5
1	H	109	ILE	2.5
1	G	94	PHE	2.5
1	H	188	GLY	2.5
1	H	52	SER	2.5
1	H	53	SER	2.5
1	G	92	ASN	2.5
1	H	305	GLU	2.5
1	A	177[A]	LYS	2.5
1	G	69	SER	2.5
1	G	90	LYS	2.5
1	G	66	VAL	2.5
1	H	232	VAL	2.5
1	H	153	PRO	2.5
1	H	123	ILE	2.4
1	G	47	HIS	2.4
1	G	19	ALA	2.4
1	H	127	TYR	2.4
1	H	51	PHE	2.4
1	H	294	ALA	2.4
1	H	207	VAL	2.4
1	G	304	ILE	2.4
1	F	51[A]	PHE	2.4
1	H	126	GLY	2.4
1	G	153	PRO	2.4
1	G	34	LYS	2.4
1	H	98	LEU	2.3
1	B	298	ASP	2.3
1	G	98	LEU	2.3
1	H	22	GLN	2.3
1	G	168	ALA	2.3
1	H	70	LYS	2.3
1	H	65	ILE	2.3
1	H	181	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	29	THR	2.3
1	H	297	ASN	2.3
1	G	314	ILE	2.3
1	H	272	ALA	2.3
1	G	133	THR	2.2
1	H	269	PHE	2.2
1	G	154	TYR	2.2
1	E	296	GLY	2.2
1	H	257	LEU	2.2
1	G	194	SER	2.2
1	H	309	PHE	2.2
1	H	154	TYR	2.2
1	G	299	ALA	2.2
1	H	172	ALA	2.2
1	G	9	ILE	2.2
1	H	40	SER	2.2
1	G	132	ASN	2.2
1	G	30	LEU	2.2
1	G	159	VAL	2.2
1	G	220	VAL	2.2
1	B	299	ALA	2.2
1	G	123	ILE	2.2
1	G	68	GLU	2.2
1	H	110	THR	2.2
1	A	47[A]	HIS	2.1
1	H	94	PHE	2.1
1	H	155	PHE	2.1
1	H	214	MET	2.1
1	H	84	VAL	2.1
1	H	156	ASP	2.1
1	G	261	GLY	2.1
1	G	57	LEU	2.1
1	H	159	VAL	2.1
1	G	167	SER	2.1
1	H	18	ALA	2.1
1	H	224	THR	2.1
1	H	296	GLY	2.1
1	H	173	LEU	2.1
1	G	97	VAL	2.1
1	F	60	GLY	2.1
1	G	10	GLY	2.1
1	G	15	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	254	TYR	2.1
1	H	189	GLY	2.1
1	G	152	HIS	2.1
1	H	57	LEU	2.1
1	H	165	LYS	2.1
1	H	199	ILE	2.1
1	H	44	TYR	2.1
1	H	125	THR	2.1
1	G	2	GLN	2.1
1	G	287	CYS	2.1
1	H	163	GLY	2.0
1	G	48	GLN	2.0
1	A	267	ASN	2.0
1	H	292	VAL	2.0
1	G	223	ILE	2.0
1	H	60	GLY	2.0
1	G	116	TYR	2.0
1	G	122	THR	2.0
1	H	282	THR	2.0
1	H	301	THR	2.0
1	E	322	LYS	2.0
1	G	310	HIS	2.0
1	H	152	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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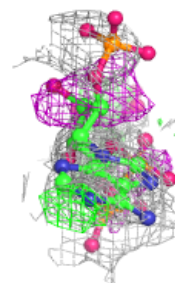
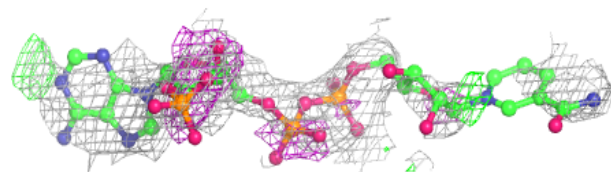
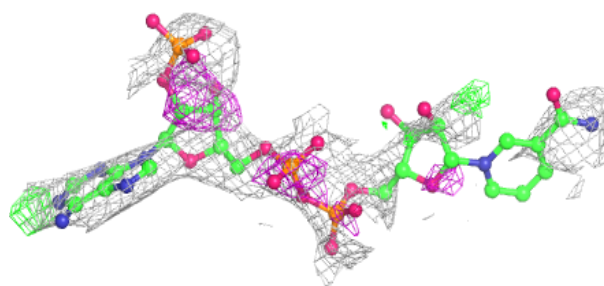
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	F	402[A]	48/48	0.51	0.24	54,72,83,87	48
3	NAP	F	402[B]	48/48	0.51	0.24	52,72,83,89	48
2	FAD	H	401	53/53	0.53	0.20	102,127,143,158	0
3	NAP	D	402[A]	48/48	0.58	0.27	45,70,82,89	48
3	NAP	D	402[B]	48/48	0.58	0.27	49,72,82,86	48
2	FAD	G	401	53/53	0.69	0.20	93,121,137,150	0
3	NAP	C	402	48/48	0.85	0.11	50,67,79,85	0
2	FAD	A	401	53/53	0.93	0.09	42,51,61,63	0
2	FAD	B	401	53/53	0.94	0.09	40,52,68,87	0
2	FAD	F	401	53/53	0.95	0.09	36,48,58,67	0
2	FAD	D	401	53/53	0.95	0.08	28,40,48,55	0
2	FAD	C	401	53/53	0.96	0.08	30,41,52,54	0
2	FAD	E	401	53/53	0.96	0.07	30,39,48,51	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.

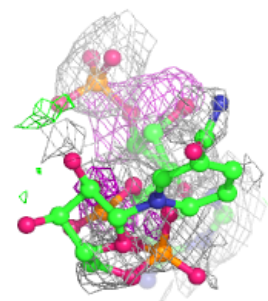
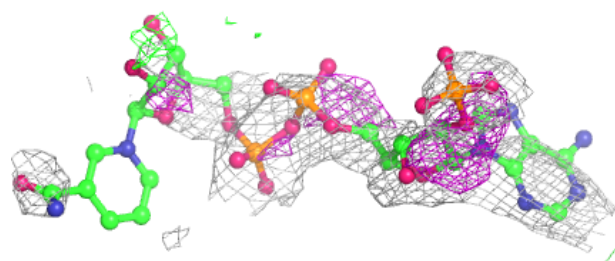
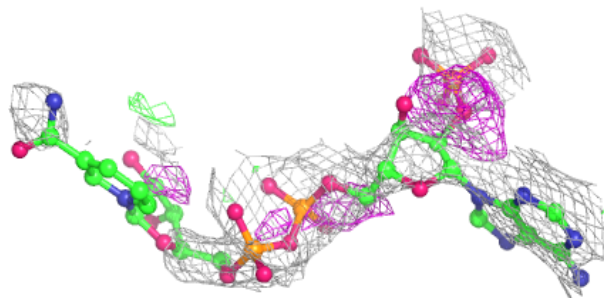
Electron density around NAP F 402 (A):

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

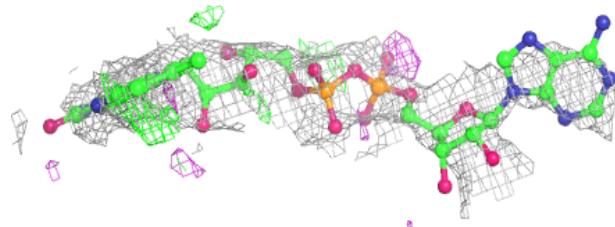
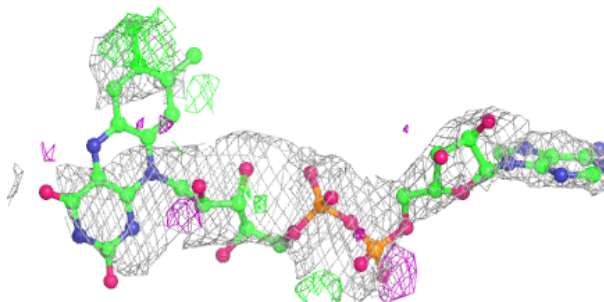


Electron density around NAP F 402 (B):

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

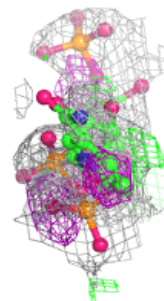
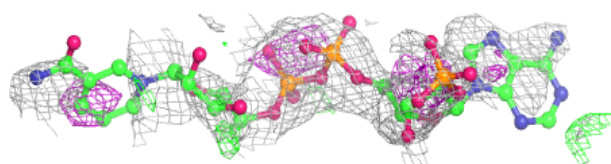
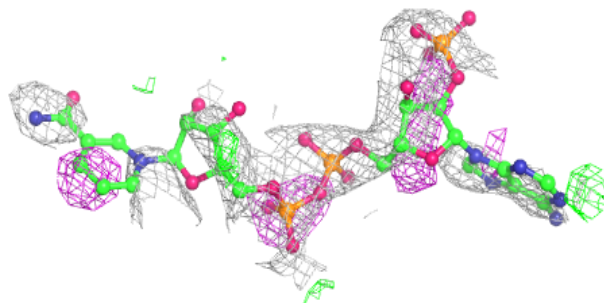
**Electron density around FAD H 401:**

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

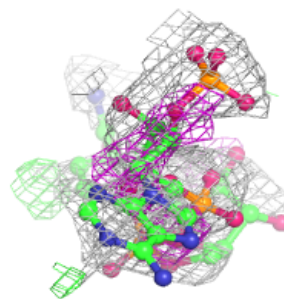
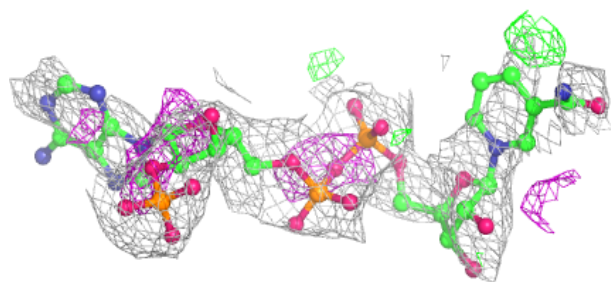
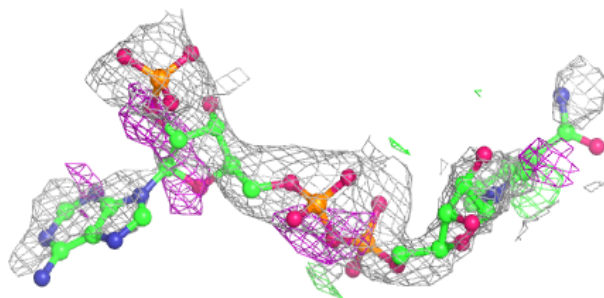


Electron density around NAP D 402 (A):

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

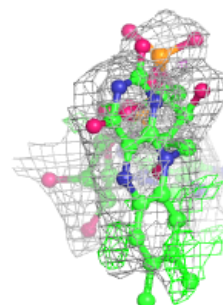
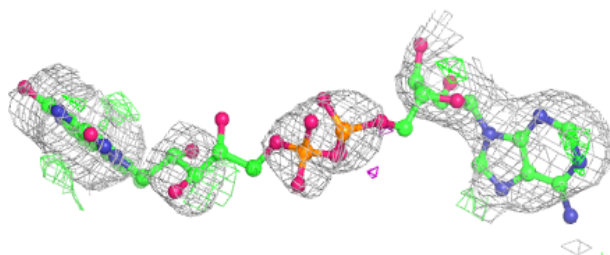
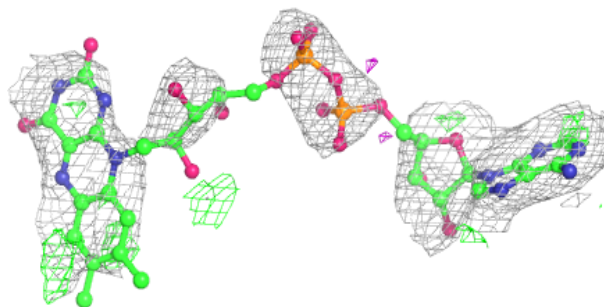
**Electron density around NAP D 402 (B):**

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

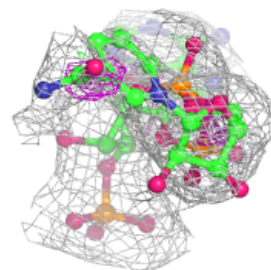
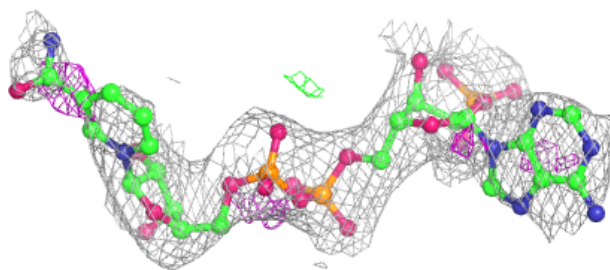
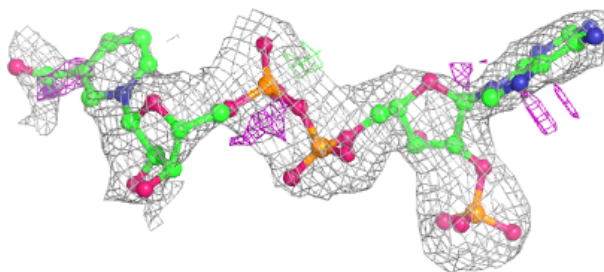


Electron density around FAD G 401:

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

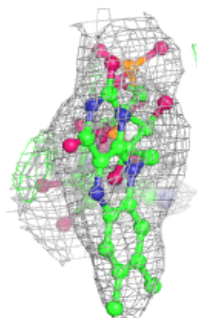
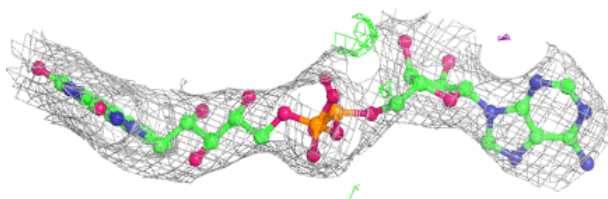
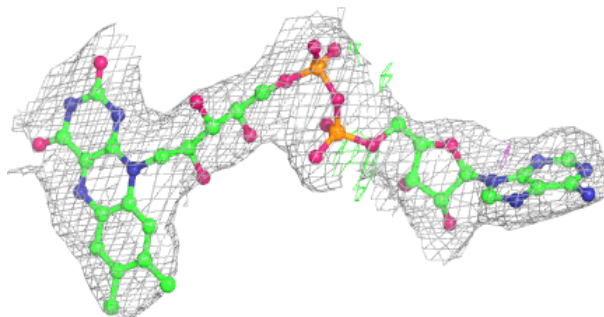
**Electron density around NAP C 402:**

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

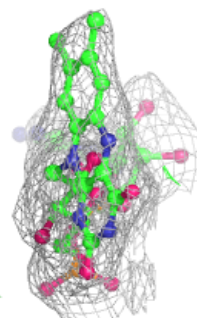
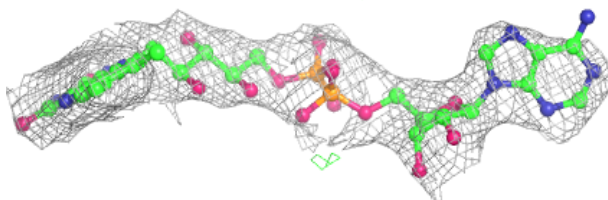
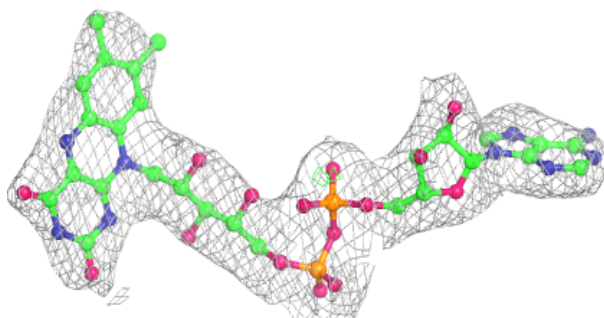


Electron density around FAD A 401:

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

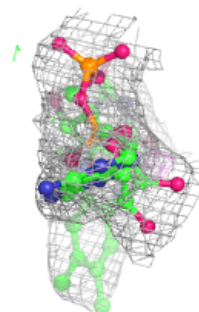
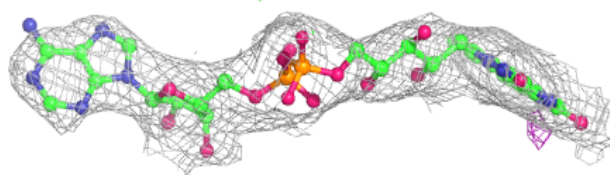
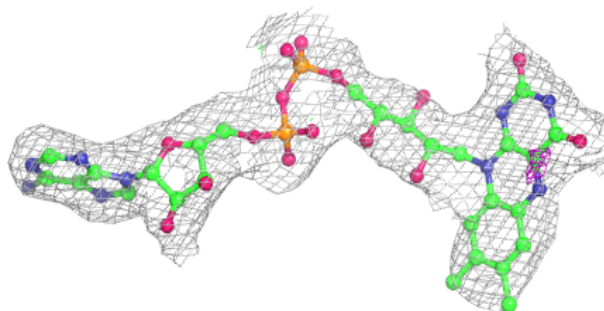
**Electron density around FAD B 401:**

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

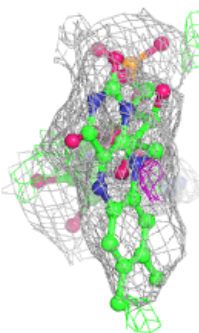
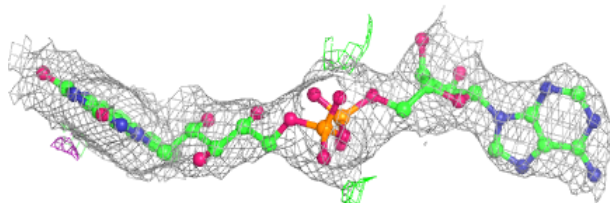
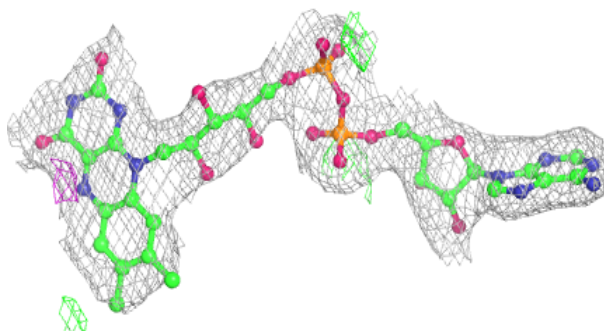


Electron density around FAD F 401:

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

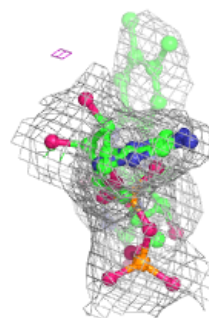
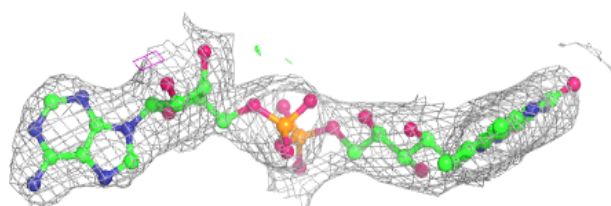
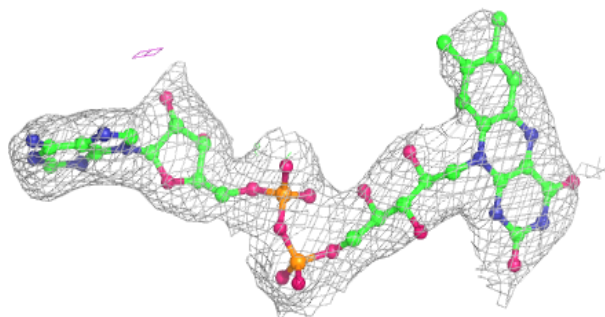
**Electron density around FAD D 401:**

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

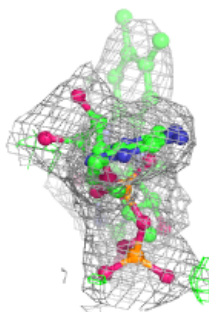
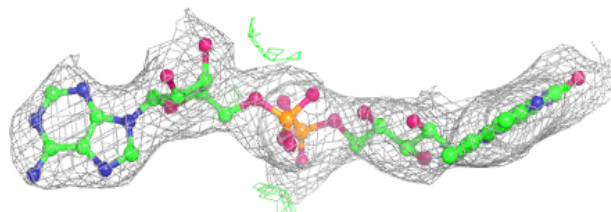
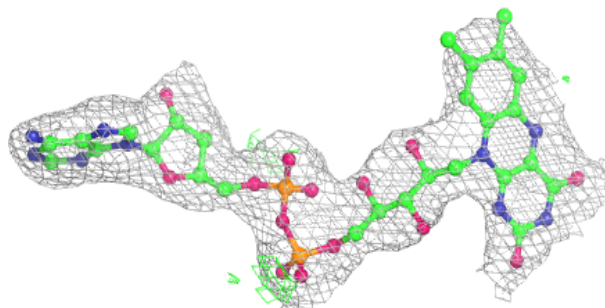


Electron density around FAD C 401:

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

**Electron density around FAD E 401:**

$2mF_o-DF_c$ (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.