



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 07:56 AM EDT

PDB ID : 1JA1
Title : CYPOR-Triple Mutant
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Deposited on : 2001-05-29
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

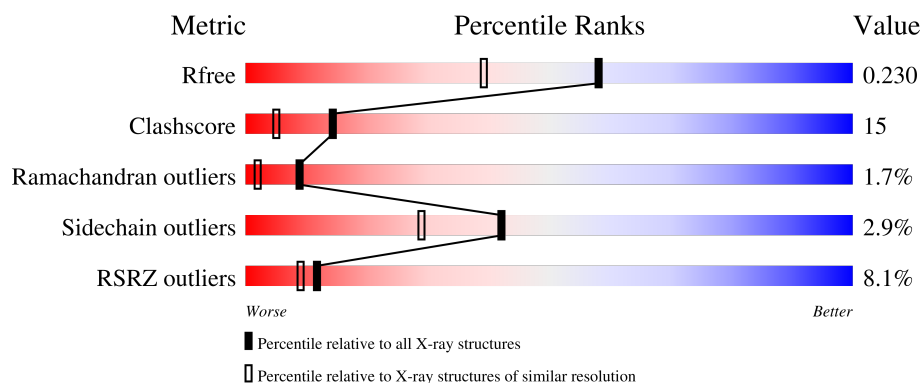
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	622	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>..</div> </div> </div>
1	B	622	<div> <div>12%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11251 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.

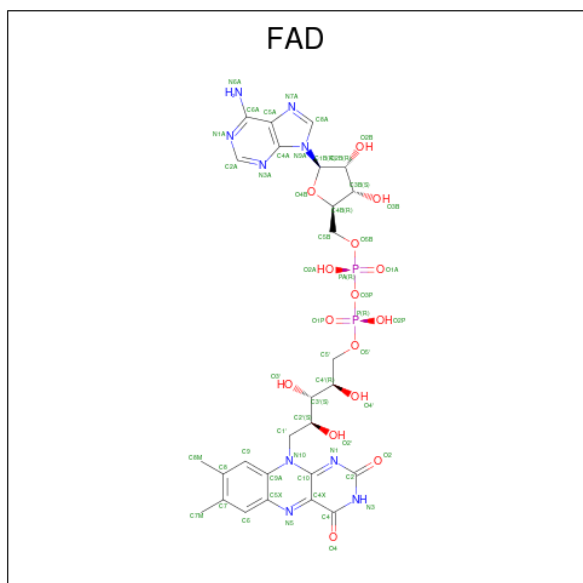
- Molecule 1 is a protein called NADPH-Cytochrome P450 Reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	616	Total	C	N	O	S	0	0	0
			4930	3119	850	939	22			
1	B	614	Total	C	N	O	S	0	0	0
			4916	3109	848	937	22			

There are 6 discrepancies between the modelled and reference sequences:

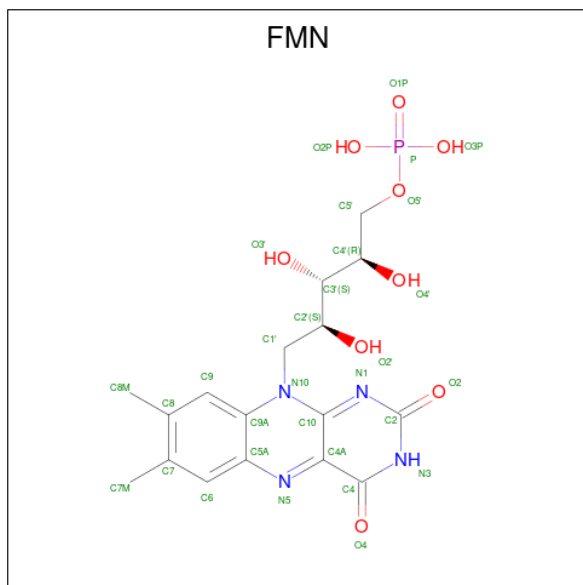
Chain	Residue	Modelled	Actual	Comment	Reference
A	457	ALA	SER	engineered mutation	UNP P00388
A	630	ALA	CYS	engineered mutation	UNP P00388
A	675	ASN	ASP	engineered mutation	UNP P00388
B	457	ALA	SER	engineered mutation	UNP P00388
B	630	ALA	CYS	engineered mutation	UNP P00388
B	675	ASN	ASP	engineered mutation	UNP P00388

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



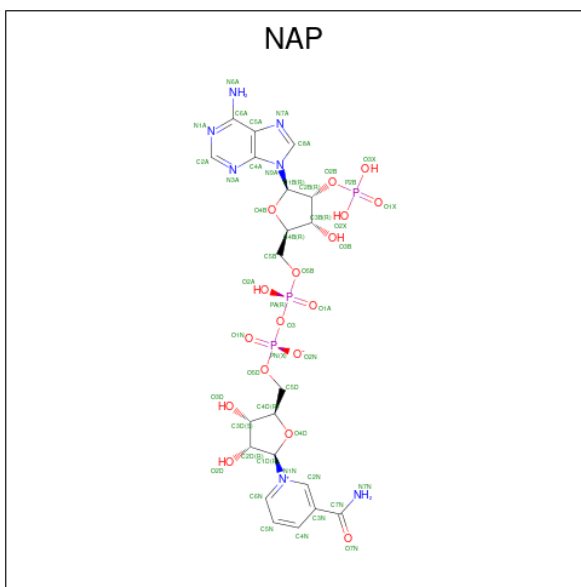
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



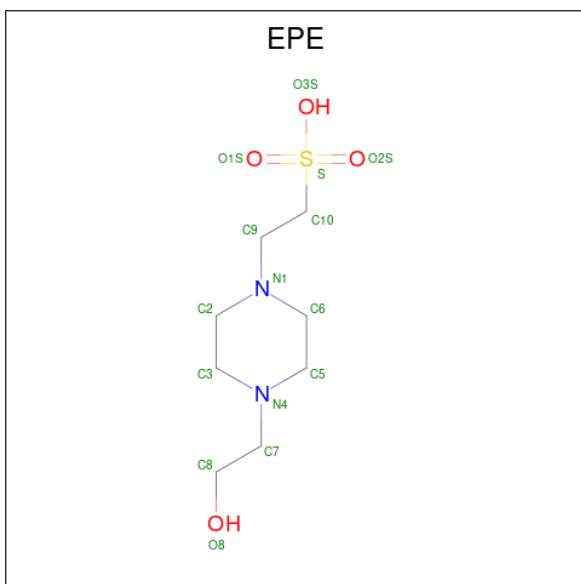
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

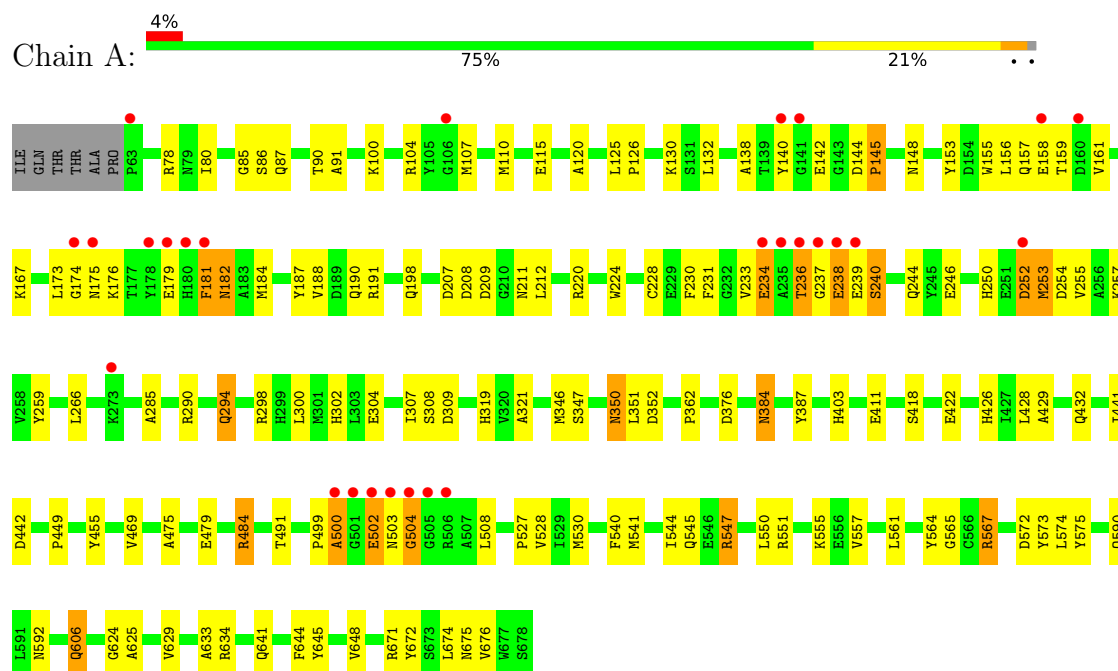
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	652	Total 652	O 652	0	0
6	B	474	Total 474	O 474	0	0

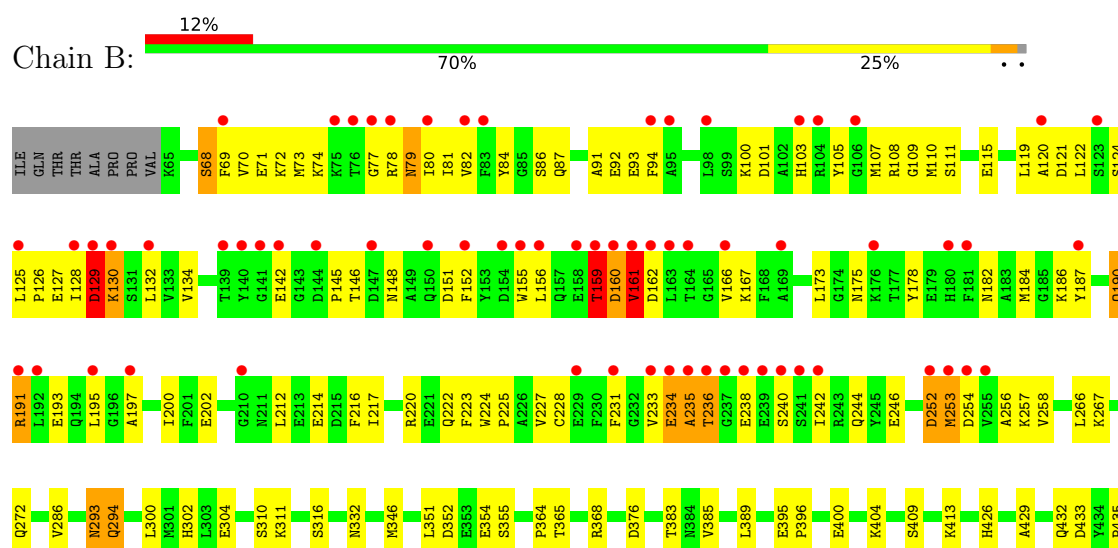
3 Residue-property plots

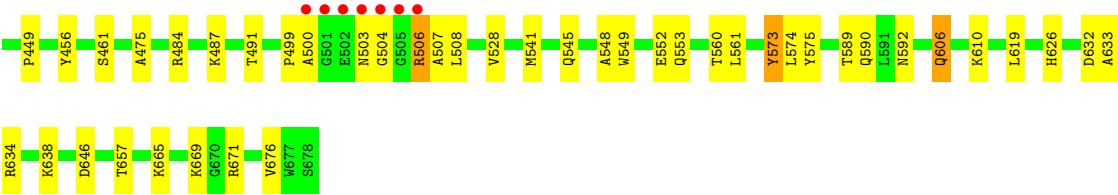
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NADPH-Cytochrome P450 Reductase



• Molecule 1: NADPH-Cytochrome P450 Reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.44Å 115.16Å 118.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.16 – 1.80 29.16 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.3 (29.16-1.80) 93.2 (29.16-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 1.79Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.234 0.203 , 0.230	Depositor DCC
R_{free} test set	6070 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11251	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, FMN, 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	0.35	0/5048	0.61	1/6831 (0.0%)
1	B	0.36	1/5033 (0.0%)	0.64	3/6810 (0.0%)
All	All	0.35	1/10081 (0.0%)	0.62	4/13641 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	ASP	CB-CG	7.32	1.67	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	LYS	N-CA-C	-6.96	92.20	111.00
1	B	159	THR	N-CA-C	6.96	129.79	111.00
1	A	85	GLY	N-CA-C	-5.42	99.55	113.10
1	B	161	VAL	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	456	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4930	0	4773	132	0
1	B	4916	0	4756	174	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	31	0	19	1	0
3	B	31	0	19	0	0
4	A	48	0	25	3	0
4	B	48	0	25	2	0
5	B	15	0	17	0	0
6	A	652	0	0	12	0
6	B	474	0	0	13	0
All	All	11251	0	9696	307	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 15.

All (307) 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:B:191:ARG:HH11	1:B:195:LEU:HD11	0.99	1.07
1:B:132:LEU:CD1	1:B:167:LYS:HB3	1.84	1.06
1:B:132:LEU:HD12	1:B:167:LYS:CB	1.86	1.06
1:B:132:LEU:HD12	1:B:167:LYS:HB3	1.06	1.03
1:A:175:ASN:O	1:A:181:PHE:HB2	1.59	1.00
1:A:606:GLN:H	1:A:606:GLN:HE21	1.01	0.99
1:B:68:SER:OG	1:B:71:GLU:HB2	1.64	0.98
1:B:606:GLN:H	1:B:606:GLN:HE21	1.08	0.97
1:A:257:LYS:HA	1:A:266:LEU:HD21	1.46	0.97
1:B:79:ASN:HD21	1:B:107:MET:HB3	1.26	0.96
1:B:74:LYS:HG2	1:B:128:ILE:HD11	1.45	0.95
1:B:167:LYS:HG3	1:B:200:ILE:HD11	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:NH1	1:B:195:LEU:HD11	1.85	0.91
1:A:606:GLN:HE22	4:A:1752:NAP:H2A	1.33	0.90
1:B:72:LYS:HD2	1:B:354:GLU:HB3	1.53	0.90
1:A:176:LYS:HG3	1:A:207:ASP:OD2	1.71	0.90
1:B:606:GLN:HE22	4:B:1852:NAP:H2A	1.35	0.89
1:B:74:LYS:HE2	1:B:128:ILE:HG12	1.55	0.89
1:B:191:ARG:HH11	1:B:195:LEU:CD1	1.86	0.88
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.54	0.87
1:B:191:ARG:O	1:B:195:LEU:HD13	1.73	0.87
1:A:175:ASN:OD1	1:A:176:LYS:N	2.07	0.86
1:B:79:ASN:ND2	1:B:107:MET:HB3	1.90	0.86
1:B:504:GLY:H	1:B:508:LEU:HD21	1.40	0.85
1:B:132:LEU:HD11	1:B:200:ILE:HG13	1.61	0.83
1:B:293:ASN:HD22	1:B:293:ASN:H	1.26	0.82
1:B:132:LEU:CD1	1:B:200:ILE:HG13	2.10	0.82
1:A:606:GLN:HE21	1:A:606:GLN:N	1.78	0.81
1:A:606:GLN:H	1:A:606:GLN:NE2	1.77	0.81
1:A:104:ARG:HH12	1:A:220:ARG:NH2	1.79	0.80
1:A:294:GLN:H	1:A:294:GLN:NE2	1.78	0.80
1:A:175:ASN:N	1:A:181:PHE:HD1	1.79	0.80
1:B:256:ALA:O	1:B:267:LYS:NZ	2.15	0.79
1:B:606:GLN:HE21	1:B:606:GLN:N	1.81	0.78
1:B:161:VAL:HG22	1:B:162:ASP:N	1.98	0.76
1:B:130:LYS:HB3	1:B:231:PHE:CD1	2.21	0.76
1:B:74:LYS:CE	1:B:128:ILE:HG12	2.16	0.76
1:B:233:VAL:O	1:B:235:ALA:N	2.17	0.76
1:B:432:GLN:HE21	1:B:484:ARG:HH21	1.33	0.76
1:B:606:GLN:H	1:B:606:GLN:NE2	1.83	0.75
1:A:298:ARG:NH2	4:A:1752:NAP:O1N	2.20	0.74
1:A:175:ASN:O	1:A:181:PHE:CD1	2.42	0.72
1:A:100:LYS:HE2	1:A:244:GLN:OE1	1.89	0.72
1:B:124:SER:O	1:B:127:GLU:HB2	1.90	0.72
1:A:175:ASN:O	1:A:181:PHE:CB	2.39	0.71
1:B:132:LEU:HD11	1:B:200:ILE:CG1	2.19	0.70
1:A:174:GLY:HA3	1:A:182:ASN:CG	2.11	0.70
1:B:161:VAL:CG2	1:B:162:ASP:H	2.05	0.69
1:B:82:VAL:HG22	1:B:134:VAL:HB	1.74	0.68
1:A:302:HIS:HD2	1:A:575:TYR:OH	1.76	0.68
1:B:69:PHE:CE1	1:B:121:ASP:HB2	2.29	0.67
1:B:128:ILE:HG22	1:B:129:ASP:N	2.09	0.67
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:VAL:CG2	1:B:162:ASP:N	2.57	0.66
1:A:257:LYS:HB2	6:A:2283:HOH:O	1.95	0.66
1:B:77:GLY:O	1:B:108:ARG:HD2	1.96	0.66
1:B:610:LYS:HZ3	1:B:646:ASP:CG	1.98	0.66
1:A:107:MET:CE	1:A:224:TRP:HZ3	2.09	0.65
1:B:78:ARG:NH1	1:B:352:ASP:OD2	2.30	0.65
1:B:252:ASP:OD2	1:B:253:MET:HB3	1.97	0.65
1:B:632:ASP:OD2	1:B:634:ARG:HG2	1.97	0.64
1:B:228:CYS:HA	1:B:233:VAL:HB	1.78	0.64
1:B:155:TRP:CZ2	1:B:160:ASP:HB3	2.33	0.64
1:A:551:ARG:HG3	1:A:557:VAL:HG21	1.81	0.63
1:A:246:GLU:HB3	1:A:351:LEU:HD21	1.81	0.63
1:B:152:PHE:HE1	1:B:156:LEU:HD21	1.63	0.63
1:A:629:VAL:HB	1:A:674:LEU:HD23	1.80	0.63
1:B:72:LYS:CD	1:B:354:GLU:HB3	2.25	0.63
1:B:126:PRO:HD3	1:B:166:VAL:HG22	1.80	0.63
1:B:145:PRO:HB3	1:B:184:MET:SD	2.39	0.63
1:B:549:TRP:O	1:B:553:GLN:HG2	1.99	0.63
1:B:252:ASP:OD2	1:B:253:MET:N	2.32	0.62
1:B:233:VAL:C	1:B:235:ALA:H	2.02	0.62
1:B:302:HIS:HD2	1:B:575:TYR:OH	1.82	0.62
1:A:140:TYR:HD2	6:A:2311:HOH:O	1.83	0.62
1:A:175:ASN:N	1:A:181:PHE:CD1	2.66	0.62
1:B:504:GLY:HA2	1:B:508:LEU:HD11	1.82	0.62
1:B:70:VAL:HG11	1:B:124:SER:O	1.98	0.61
1:B:233:VAL:O	1:B:233:VAL:HG12	1.98	0.61
1:B:82:VAL:O	1:B:111:SER:HA	2.00	0.61
1:B:606:GLN:NE2	4:B:1852:NAP:H2A	2.13	0.61
1:A:104:ARG:NH1	1:A:220:ARG:NH2	2.48	0.61
1:B:79:ASN:HD21	1:B:107:MET:CB	2.09	0.61
1:B:161:VAL:HG22	1:B:162:ASP:H	1.65	0.61
1:B:561:LEU:HD22	1:B:590:GLN:HB2	1.82	0.61
1:B:504:GLY:H	1:B:508:LEU:CD2	2.12	0.61
1:A:590:GLN:HE21	1:A:592:ASN:HD21	1.48	0.61
1:A:157:GLN:HB2	1:A:158:GLU:OE1	2.01	0.60
1:A:209:ASP:OD1	1:A:634:ARG:NH2	2.34	0.60
1:A:236:THR:O	1:A:238:GLU:HG3	2.01	0.60
1:B:87:GLN:HG3	1:B:146:THR:HG22	1.84	0.60
1:B:235:ALA:O	1:B:236:THR:HG23	2.00	0.59
1:A:228:CYS:HA	1:A:233:VAL:CG2	2.32	0.59
1:B:115:GLU:OE1	1:B:148:ASN:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:SER:HA	1:B:413:LYS:HD3	1.84	0.59
1:B:426:HIS:CD2	1:B:429:ALA:H	2.20	0.59
1:A:107:MET:HE1	1:A:224:TRP:HZ3	1.67	0.59
1:A:175:ASN:H	1:A:181:PHE:HD1	1.49	0.59
1:B:220:ARG:HD3	6:B:2138:HOH:O	2.03	0.58
1:A:319:HIS:HD2	6:A:1865:HOH:O	1.86	0.58
1:B:70:VAL:HA	1:B:73:MET:HE3	1.84	0.58
1:A:376:ASP:HB3	1:A:449:PRO:HG2	1.84	0.58
1:B:80:ILE:O	1:B:109:GLY:HA2	2.02	0.58
1:A:228:CYS:HA	1:A:233:VAL:HG22	1.86	0.58
1:B:80:ILE:HD11	1:B:107:MET:CE	2.33	0.58
1:B:81:ILE:HA	1:B:110:MET:O	2.03	0.58
1:B:638:LYS:NZ	6:B:2307:HOH:O	2.36	0.58
1:B:294:GLN:HE22	1:B:573:TYR:H	1.51	0.57
1:B:432:GLN:NE2	1:B:484:ARG:HH21	2.01	0.57
1:B:426:HIS:HD2	1:B:429:ALA:H	1.52	0.57
1:B:128:ILE:CG2	1:B:129:ASP:N	2.67	0.57
1:B:300:LEU:HD22	1:B:574:LEU:HD21	1.86	0.57
1:B:504:GLY:N	1:B:508:LEU:HD21	2.16	0.57
1:A:254:ASP:O	1:A:257:LYS:HG2	2.03	0.57
1:A:384:ASN:HD22	1:A:384:ASN:H	1.51	0.57
1:A:174:GLY:CA	1:A:182:ASN:ND2	2.69	0.56
1:B:70:VAL:HA	1:B:73:MET:CE	2.34	0.56
1:B:223:PHE:O	1:B:227:VAL:HG23	2.06	0.56
1:B:234:GLU:O	1:B:235:ALA:HB3	2.05	0.56
1:A:174:GLY:HA3	1:A:182:ASN:ND2	2.21	0.56
1:A:294:GLN:H	1:A:294:GLN:HE21	1.52	0.56
1:B:125:LEU:N	1:B:126:PRO:HD2	2.20	0.56
1:B:294:GLN:H	1:B:294:GLN:NE2	2.03	0.56
1:A:500:ALA:HB1	1:A:504:GLY:O	2.06	0.56
1:A:78:ARG:CD	1:A:110:MET:HB3	2.36	0.55
1:B:231:PHE:HB2	1:B:233:VAL:HG23	1.87	0.55
1:B:548:ALA:O	1:B:552:GLU:HG2	2.07	0.55
1:A:157:GLN:HG2	1:A:187:TYR:OH	2.07	0.55
1:B:234:GLU:O	1:B:235:ALA:CB	2.55	0.55
1:B:78:ARG:HH12	1:B:352:ASP:HB2	1.72	0.55
1:A:350:ASN:HD22	1:A:352:ASP:H	1.54	0.55
1:B:128:ILE:O	1:B:129:ASP:O	2.25	0.55
1:B:152:PHE:CE1	1:B:156:LEU:HD21	2.42	0.55
1:B:385:VAL:O	1:B:389:LEU:HG	2.07	0.55
1:B:590:GLN:HE21	1:B:592:ASN:HD21	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:LEU:HD22	1:A:555:LYS:HD2	1.89	0.55
1:B:665:LYS:HE2	1:B:669:LYS:NZ	2.22	0.55
1:A:237:GLY:O	1:A:239:GLU:N	2.41	0.54
1:B:119:LEU:O	1:B:122:LEU:HG	2.07	0.54
1:A:87:GLN:NE2	1:A:140:TYR:CE2	2.76	0.54
1:A:174:GLY:N	1:A:182:ASN:ND2	2.55	0.54
1:A:350:ASN:ND2	1:A:352:ASP:H	2.06	0.53
1:A:174:GLY:O	1:A:207:ASP:HA	2.09	0.53
1:B:395:GLU:OE1	1:B:396:PRO:HD2	2.09	0.53
1:A:633:ALA:HB2	1:A:676:VAL:HB	1.90	0.52
1:B:214:GLU:OE1	1:B:413:LYS:HE3	2.10	0.52
1:A:321:ALA:HB2	1:A:455:TYR:CE1	2.44	0.52
1:A:541:MET:O	1:A:545:GLN:HG3	2.08	0.52
1:B:187:TYR:CZ	1:B:191:ARG:HG3	2.44	0.52
1:B:316:SER:OG	1:B:461:SER:HA	2.10	0.52
1:B:73:MET:HB3	1:B:78:ARG:O	2.10	0.52
1:B:426:HIS:HE1	6:B:2021:HOH:O	1.92	0.52
1:B:293:ASN:HD22	1:B:293:ASN:N	1.99	0.52
1:A:499:PRO:O	1:A:500:ALA:HB3	2.09	0.52
1:B:120:ALA:HA	1:B:155:TRP:CZ2	2.45	0.52
1:B:503:ASN:HB2	6:B:2155:HOH:O	2.09	0.52
1:B:610:LYS:NZ	1:B:646:ASP:CG	2.62	0.52
1:A:115:GLU:OE1	1:A:148:ASN:HA	2.10	0.52
1:B:665:LYS:HD3	6:B:2158:HOH:O	2.09	0.52
1:A:78:ARG:NE	1:A:110:MET:HB3	2.25	0.51
1:A:350:ASN:HD22	1:A:351:LEU:N	2.08	0.51
1:A:175:ASN:OD1	1:A:209:ASP:HB2	2.11	0.51
1:B:93:GLU:HG3	6:B:2160:HOH:O	2.10	0.51
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.93	0.51
1:A:298:ARG:HD2	6:A:1830:HOH:O	2.11	0.51
1:B:191:ARG:CD	1:B:195:LEU:HD11	2.41	0.51
1:B:657:THR:HG23	6:B:2097:HOH:O	2.11	0.51
1:B:217:ILE:HG23	6:B:2287:HOH:O	2.11	0.51
1:B:254:ASP:OD1	1:B:257:LYS:HG3	2.11	0.51
1:A:184:MET:HE2	1:A:184:MET:O	2.10	0.51
1:A:145:PRO:HG2	1:A:153:TYR:CG	2.46	0.51
1:B:175:ASN:HB3	1:B:178:TYR:CD2	2.46	0.50
1:A:606:GLN:NE2	4:A:1752:NAP:H2A	2.16	0.50
1:B:186:LYS:O	1:B:190:GLN:HB2	2.12	0.50
1:B:266:LEU:O	1:B:267:LYS:HB2	2.10	0.50
1:B:79:ASN:N	1:B:79:ASN:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:CG	1:A:176:LYS:H	2.06	0.50
1:B:125:LEU:C	1:B:127:GLU:H	2.15	0.50
1:A:87:GLN:NE2	1:A:140:TYR:CZ	2.80	0.50
1:A:211:ASN:HA	6:A:2116:HOH:O	2.11	0.50
1:A:290:ARG:HD3	6:A:2384:HOH:O	2.11	0.50
1:A:302:HIS:HE1	1:A:304:GLU:OE1	1.95	0.50
1:B:159:THR:O	1:B:160:ASP:CB	2.59	0.50
1:B:175:ASN:HB3	1:B:178:TYR:HD2	1.76	0.50
1:B:125:LEU:HD23	1:B:166:VAL:HG13	1.92	0.50
1:B:310:SER:O	1:B:311:LYS:HB2	2.10	0.49
1:B:193:GLU:HA	1:B:197:ALA:O	2.13	0.49
1:A:175:ASN:O	1:A:181:PHE:CG	2.64	0.49
1:B:217:ILE:HD11	1:B:383:THR:HG21	1.93	0.49
1:A:184:MET:HA	1:A:184:MET:CE	2.42	0.49
1:B:68:SER:HG	1:B:71:GLU:HB2	1.75	0.49
1:B:159:THR:O	1:B:160:ASP:HB3	2.12	0.49
1:B:125:LEU:C	1:B:127:GLU:N	2.64	0.49
1:A:479:GLU:HB3	6:A:2229:HOH:O	2.13	0.49
1:A:175:ASN:C	1:A:176:LYS:HG2	2.34	0.48
1:B:400:GLU:CD	1:B:404:LYS:HE3	2.33	0.48
1:B:302:HIS:HE1	1:B:304:GLU:OE1	1.96	0.48
2:B:1850:FAD:HM73	6:B:1961:HOH:O	2.14	0.48
1:B:500:ALA:HB3	6:B:2178:HOH:O	2.13	0.48
1:B:246:GLU:HB2	1:B:351:LEU:HD21	1.96	0.48
1:B:541:MET:O	1:B:545:GLN:HG3	2.13	0.48
1:A:624:GLY:HA2	1:A:671:ARG:NH2	2.29	0.48
1:B:222:GLN:C	1:B:225:PRO:HD2	2.35	0.47
1:B:396:PRO:HG2	6:B:2277:HOH:O	2.13	0.47
1:A:426:HIS:HD2	1:A:429:ALA:H	1.62	0.47
1:B:293:ASN:ND2	1:B:300:LEU:H	2.12	0.47
1:A:527:PRO:HB2	1:A:625:ALA:HB2	1.97	0.47
1:A:567:ARG:HG2	1:A:572:ASP:OD2	2.15	0.47
1:B:80:ILE:HD11	1:B:107:MET:HE1	1.95	0.47
1:B:155:TRP:CE2	1:B:159:THR:O	2.68	0.47
1:A:125:LEU:N	1:A:126:PRO:CD	2.78	0.46
1:A:561:LEU:N	1:A:561:LEU:HD12	2.30	0.46
1:A:155:TRP:CZ2	1:A:161:VAL:HG11	2.50	0.46
1:A:250:HIS:HE1	1:A:347:SER:OG	1.98	0.46
1:B:242:ILE:O	1:B:242:ILE:HG13	2.15	0.46
1:A:403:HIS:HB2	6:A:2356:HOH:O	2.14	0.46
1:B:126:PRO:HD3	1:B:166:VAL:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:PHE:O	1:B:72:LYS:HB3	2.15	0.46
1:A:130:LYS:HA	1:A:231:PHE:CE1	2.50	0.46
1:A:239:GLU:O	1:A:240:SER:HB3	2.16	0.46
1:A:564:TYR:CG	1:A:565:GLY:N	2.83	0.46
1:B:475:ALA:HA	1:B:491:THR:HB	1.97	0.46
1:B:173:LEU:N	1:B:173:LEU:HD12	2.31	0.46
1:B:272:GLN:HA	6:B:1949:HOH:O	2.17	0.46
1:A:78:ARG:HD3	1:A:110:MET:HB3	1.97	0.45
1:B:233:VAL:O	1:B:233:VAL:CG1	2.63	0.45
1:A:90:THR:HG21	1:A:212:LEU:HD23	1.97	0.45
1:B:238:GLU:O	1:B:240:SER:N	2.50	0.45
1:A:300:LEU:HD22	1:A:574:LEU:HD21	1.99	0.45
1:A:120:ALA:HA	1:A:155:TRP:CZ2	2.52	0.45
1:A:174:GLY:N	1:A:182:ASN:HD21	2.15	0.45
1:A:253:MET:CE	1:A:257:LYS:HG3	2.46	0.45
1:A:175:ASN:CA	1:A:181:PHE:HD1	2.29	0.44
1:B:236:THR:HB	1:B:238:GLU:HG3	1.99	0.44
1:A:107:MET:CE	1:A:224:TRP:CZ3	2.96	0.44
1:A:426:HIS:CD2	1:A:429:ALA:H	2.34	0.44
1:A:644:PHE:O	1:A:648:VAL:HG23	2.18	0.44
1:B:626:HIS:CD2	1:B:671:ARG:HG2	2.53	0.44
1:A:175:ASN:CG	1:A:176:LYS:N	2.63	0.44
1:A:590:GLN:NE2	1:A:592:ASN:HD21	2.14	0.44
1:B:101:ASP:HB2	1:B:224:TRP:CZ2	2.53	0.44
1:B:142:GLU:N	1:B:142:GLU:OE1	2.50	0.44
1:B:159:THR:HG22	1:B:191:ARG:NH1	2.33	0.44
1:B:506:ARG:O	1:B:508:LEU:HG	2.17	0.44
1:A:319:HIS:HE1	1:A:675:ASN:OD1	2.00	0.44
1:A:528:VAL:HG12	1:A:530:MET:HG3	2.00	0.44
1:A:239:GLU:CD	1:A:387:TYR:HH	2.22	0.43
1:B:100:LYS:HG2	1:B:244:GLN:OE1	2.18	0.43
1:B:120:ALA:HB1	1:B:160:ASP:OD2	2.18	0.43
1:B:78:ARG:HH22	1:B:352:ASP:HB2	1.83	0.43
1:A:159:THR:OG1	1:A:161:VAL:HG12	2.17	0.43
1:A:140:TYR:CZ	3:A:1751:FMN:HM73	2.54	0.43
1:A:138:ALA:HA	1:A:173:LEU:HB2	2.00	0.43
1:B:235:ALA:O	1:B:236:THR:OG1	2.35	0.43
1:A:175:ASN:OD1	1:A:207:ASP:OD1	2.37	0.43
1:A:198:GLN:NE2	6:A:2272:HOH:O	2.48	0.43
1:B:103:HIS:C	1:B:105:TYR:H	2.22	0.43
1:B:182:ASN:O	1:B:186:LYS:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:H	1:B:293:ASN:ND2	2.04	0.42
1:A:175:ASN:O	1:A:181:PHE:HD1	2.00	0.42
1:A:484:ARG:N	1:A:484:ARG:HD2	2.34	0.42
1:B:487:LYS:CE	6:B:1943:HOH:O	2.66	0.42
1:A:80:ILE:HD12	1:A:132:LEU:HD23	2.00	0.42
1:B:352:ASP:OD1	1:B:352:ASP:C	2.57	0.42
1:A:184:MET:HE2	1:A:188:VAL:HG23	2.00	0.42
1:B:84:TYR:CD2	1:B:92:GLU:HB2	2.54	0.42
1:A:182:ASN:HD22	1:A:182:ASN:HA	1.63	0.42
1:A:502:GLU:C	1:A:503:ASN:HD22	2.23	0.42
1:A:567:ARG:HG2	1:A:567:ARG:H	1.55	0.42
1:A:551:ARG:NH1	6:A:2362:HOH:O	2.48	0.42
1:B:253:MET:SD	1:B:364:PRO:HG3	2.60	0.42
1:B:286:VAL:O	1:B:499:PRO:HA	2.20	0.42
1:B:332:ASN:ND2	1:B:368:ARG:NH1	2.67	0.42
1:A:252:ASP:OD1	1:A:253:MET:N	2.51	0.42
1:A:441:ILE:HG23	1:A:442:ASP:N	2.35	0.42
1:A:156:LEU:HB3	1:A:191:ARG:HG2	2.02	0.42
1:A:285:ALA:HA	1:A:508:LEU:HD23	2.01	0.42
1:B:94:PHE:HB3	1:B:216:PHE:CE1	2.55	0.42
1:B:235:ALA:O	1:B:236:THR:CG2	2.67	0.41
1:B:258:VAL:HG13	1:B:365:THR:HA	2.01	0.41
1:A:167:LYS:HE2	1:A:230:PHE:CZ	2.54	0.41
1:A:182:ASN:ND2	6:A:2006:HOH:O	2.46	0.41
1:B:74:LYS:CG	1:B:128:ILE:HD11	2.33	0.41
1:A:259:TYR:CD2	1:A:362:PRO:HB3	2.54	0.41
1:A:540:PHE:O	1:A:544:ILE:HG13	2.21	0.41
1:A:641:GLN:NE2	1:A:645:TYR:OH	2.44	0.41
1:A:308:SER:O	1:A:309:ASP:HB2	2.21	0.41
1:B:294:GLN:HE22	1:B:573:TYR:N	2.18	0.41
1:A:100:LYS:HE2	1:A:244:GLN:CD	2.42	0.41
1:A:142:GLU:N	1:A:142:GLU:CD	2.74	0.41
1:B:233:VAL:O	1:B:234:GLU:HG3	2.21	0.41
1:B:528:VAL:HG22	1:B:560:THR:HA	2.02	0.41
1:B:561:LEU:HD23	1:B:589:THR:HB	2.03	0.41
1:B:633:ALA:HB2	1:B:676:VAL:HB	2.02	0.41
1:A:144:ASP:HA	1:A:145:PRO:HD3	1.92	0.41
1:A:547:ARG:NH1	6:A:1880:HOH:O	2.54	0.41
1:A:234:GLU:C	1:A:236:THR:H	2.25	0.40
1:B:74:LYS:HG2	1:B:128:ILE:CD1	2.33	0.40
1:A:428:LEU:O	1:A:432:GLN:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ALA:HA	1:A:491:THR:HB	2.03	0.40
1:B:79:ASN:HD21	1:B:108:ARG:H	1.69	0.40
1:B:433:ASP:C	1:B:435:PRO:HD3	2.41	0.40
1:A:307:ILE:HD13	1:A:469:VAL:HG23	2.03	0.40
1:B:235:ALA:O	1:B:236:THR:CB	2.69	0.40
1:A:418:SER:HA	1:A:422:GLU:HB3	2.02	0.40
1:B:68:SER:HB2	1:B:71:GLU:OE2	2.21	0.40
1:A:208:ASP:O	1:A:208:ASP:OD1	2.39	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	614/622 (99%)	583 (95%)	21 (3%)	10 (2%)	9	2
1	B	612/622 (98%)	573 (94%)	28 (5%)	11 (2%)	8	2
All	All	1226/1244 (99%)	1156 (94%)	49 (4%)	21 (2%)	9	2

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	THR
1	B	129	ASP
1	B	159	THR
1	B	161	VAL
1	B	234	GLU
1	B	235	ALA
1	A	240	SER
1	A	253	MET
1	B	160	ASP
1	B	202	GLU

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Mol	Chain	Res	Type
1	B	236	THR
1	A	179	GLU
1	A	238	GLU
1	A	500	ALA
1	B	507	ALA
1	A	502	GLU
1	B	506	ARG
1	B	68	SER
1	A	504	GLY
1	A	145	PRO
1	A	255	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	524/529 (99%)	508 (97%)	16 (3%)	40	25
1	B	522/529 (99%)	508 (97%)	14 (3%)	44	31
All	All	1046/1058 (99%)	1016 (97%)	30 (3%)	42	29

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	PHE
1	A	182	ASN
1	A	190	GLN
1	A	234	GLU
1	A	252	ASP
1	A	294	GLN
1	A	346	MET
1	A	350	ASN
1	A	384	ASN
1	A	411	GLU
1	A	484	ARG
1	A	547	ARG

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Mol	Chain	Res	Type
1	A	567	ARG
1	A	573	TYR
1	A	606	GLN
1	A	672	TYR
1	B	79	ASN
1	B	129	ASP
1	B	151	ASP
1	B	190	GLN
1	B	191	ARG
1	B	212	LEU
1	B	253	MET
1	B	293	ASN
1	B	294	GLN
1	B	346	MET
1	B	355	SER
1	B	573	TYR
1	B	606	GLN
1	B	619	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	182	ASN
1	A	250	HIS
1	A	280	ASN
1	A	294	GLN
1	A	302	HIS
1	A	319	HIS
1	A	332	ASN
1	A	333	GLN
1	A	350	ASN
1	A	359	HIS
1	A	384	ASN
1	A	391	GLN
1	A	399	GLN
1	A	426	HIS
1	A	486	ASN
1	A	503	ASN
1	A	590	GLN
1	A	606	GLN
1	A	641	GLN

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Mol	Chain	Res	Type
1	B	79	ASN
1	B	96	ASN
1	B	280	ASN
1	B	293	ASN
1	B	294	GLN
1	B	302	HIS
1	B	332	ASN
1	B	349	ASN
1	B	359	HIS
1	B	403	HIS
1	B	426	HIS
1	B	432	GLN
1	B	467	ASN
1	B	486	ASN
1	B	583	HIS
1	B	590	GLN
1	B	606	GLN
1	B	641	GLN

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](#)

7 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	NAP	A	1752	-	45,52,52	2.17	11 (24%)	56,80,80	1.39	9 (16%)
2	FAD	A	1750	-	51,58,58	2.44	17 (33%)	60,89,89	2.79	15 (25%)
5	EPE	B	1753	-	15,15,15	1.76	3 (20%)	18,20,20	0.89	0
2	FAD	B	1850	-	51,58,58	2.42	15 (29%)	60,89,89	2.73	15 (25%)
4	NAP	B	1852	-	45,52,52	2.11	10 (22%)	56,80,80	1.41	9 (16%)
3	FMN	A	1751	-	31,33,33	2.37	11 (35%)	40,50,50	3.56	16 (40%)
3	FMN	B	1851	-	31,33,33	2.42	9 (29%)	40,50,50	3.61	17 (42%)

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	NAP	A	1752	-	-	6/31/67/67	0/5/5/5
2	FAD	A	1750	-	-	3/30/50/50	0/6/6/6
5	EPE	B	1753	-	-	1/9/19/19	0/1/1/1
2	FAD	B	1850	-	-	3/30/50/50	0/6/6/6
4	NAP	B	1852	-	-	3/31/67/67	0/5/5/5
3	FMN	A	1751	-	-	0/18/18/18	0/3/3/3
3	FMN	B	1851	-	-	0/18/18/18	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1752	NAP	C4A-N3A	8.37	1.47	1.35
4	B	1852	NAP	C4A-N3A	8.22	1.47	1.35
2	B	1850	FAD	C9A-N10	6.83	1.47	1.38
3	B	1851	FMN	C8M-C8	-6.83	1.37	1.51
2	A	1750	FAD	C9A-N10	6.77	1.47	1.38
3	A	1751	FMN	C8M-C8	-6.68	1.37	1.51
3	B	1851	FMN	C9A-N10	6.65	1.47	1.38
2	A	1750	FAD	C4X-C10	6.44	1.45	1.38
4	A	1752	NAP	C7N-N7N	6.40	1.45	1.33
4	B	1852	NAP	C7N-N7N	6.35	1.45	1.33
2	B	1850	FAD	C4X-C10	6.15	1.45	1.38
2	B	1850	FAD	C4-N3	5.38	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1750	FAD	C4-N3	4.91	1.41	1.33
3	A	1751	FMN	C4A-N5	4.82	1.40	1.33
2	A	1750	FAD	C4A-N3A	4.79	1.42	1.35
2	B	1850	FAD	C4A-N3A	4.55	1.41	1.35
2	A	1750	FAD	C10-N1	4.53	1.39	1.33
2	A	1750	FAD	C4X-N5	4.49	1.39	1.33
5	B	1753	EPE	C9-C10	-4.47	1.40	1.52
2	B	1850	FAD	C4X-N5	4.42	1.39	1.33
3	A	1751	FMN	C9A-N10	4.40	1.44	1.38
2	B	1850	FAD	C10-N1	4.32	1.38	1.33
3	A	1751	FMN	C1'-N10	-4.30	1.43	1.48
3	B	1851	FMN	C10-N1	4.26	1.38	1.33
3	B	1851	FMN	C4A-N5	4.23	1.39	1.33
2	A	1750	FAD	C2'-C3'	3.94	1.60	1.53
2	B	1850	FAD	C2'-C3'	3.85	1.60	1.53
3	B	1851	FMN	C4A-C10	3.63	1.42	1.38
2	A	1750	FAD	C4-C4X	3.57	1.47	1.41
2	A	1750	FAD	C5'-C4'	3.50	1.56	1.51
4	A	1752	NAP	C2A-N1A	3.50	1.40	1.33
2	A	1750	FAD	C5X-N5	3.48	1.41	1.35
2	B	1850	FAD	C4-C4X	3.45	1.47	1.41
2	B	1850	FAD	C5'-C4'	3.34	1.56	1.51
3	A	1751	FMN	C4-N3	3.29	1.38	1.33
4	B	1852	NAP	C2N-C3N	3.22	1.44	1.39
4	A	1752	NAP	C2N-C3N	3.21	1.44	1.39
4	B	1852	NAP	C2A-N1A	3.20	1.39	1.33
2	B	1850	FAD	C5X-N5	3.15	1.40	1.35
3	A	1751	FMN	C10-N1	3.14	1.37	1.33
4	A	1752	NAP	P2B-O1X	3.13	1.60	1.50
4	B	1852	NAP	C4N-C3N	2.97	1.44	1.39
4	B	1852	NAP	P2B-O1X	2.94	1.60	1.50
4	A	1752	NAP	C4N-C3N	2.91	1.44	1.39
2	B	1850	FAD	C2A-N3A	2.83	1.36	1.32
2	A	1750	FAD	C8-C7	2.81	1.47	1.40
2	B	1850	FAD	C8-C7	2.78	1.47	1.40
4	B	1852	NAP	O4D-C1D	2.70	1.44	1.41
2	A	1750	FAD	C9A-C5X	2.66	1.47	1.42
4	A	1752	NAP	C5A-C4A	2.57	1.47	1.40
4	A	1752	NAP	O4D-C1D	2.55	1.44	1.41
2	B	1850	FAD	O2'-C2'	2.53	1.48	1.43
2	A	1750	FAD	C6-C5X	2.50	1.45	1.41
3	A	1751	FMN	C2-N1	-2.49	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1753	EPE	C2-N1	2.49	1.53	1.46
3	A	1751	FMN	C8-C7	2.45	1.47	1.40
3	A	1751	FMN	O2'-C2'	2.44	1.48	1.43
2	A	1750	FAD	C8A-N7A	2.40	1.39	1.34
2	B	1850	FAD	C6-C5X	2.39	1.45	1.41
4	B	1852	NAP	C5A-C4A	2.38	1.47	1.40
3	B	1851	FMN	C4-N3	2.35	1.37	1.33
3	B	1851	FMN	C9-C9A	2.33	1.45	1.40
5	B	1753	EPE	C6-N1	2.32	1.53	1.46
2	A	1750	FAD	C2A-N3A	2.29	1.35	1.32
4	B	1852	NAP	C6N-N1N	2.27	1.40	1.35
3	B	1851	FMN	C8-C7	2.23	1.46	1.40
2	B	1850	FAD	C9A-C5X	2.23	1.47	1.42
4	A	1752	NAP	C6N-N1N	2.20	1.40	1.35
3	B	1851	FMN	C4'-C3'	2.18	1.57	1.53
4	A	1752	NAP	PN-O2N	-2.12	1.45	1.55
2	A	1750	FAD	C6-C7	2.12	1.43	1.37
3	A	1751	FMN	C5A-N5	2.08	1.38	1.35
4	B	1852	NAP	PN-O2N	-2.07	1.45	1.55
4	A	1752	NAP	PA-O2A	-2.05	1.45	1.55
3	A	1751	FMN	C4A-C10	2.04	1.40	1.38
2	A	1750	FAD	O2'-C2'	2.01	1.47	1.43

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1851	FMN	C4-N3-C2	15.08	127.88	115.14
3	A	1751	FMN	C4-N3-C2	14.48	127.37	115.14
2	A	1750	FAD	C4-N3-C2	14.29	127.21	115.14
2	B	1850	FAD	C4-N3-C2	14.05	127.01	115.14
3	A	1751	FMN	C10-C4A-N5	8.85	127.38	121.26
3	B	1851	FMN	C10-C4A-N5	8.55	127.17	121.26
2	A	1750	FAD	C1'-N10-C9A	8.20	124.75	118.29
2	B	1850	FAD	C1'-N10-C9A	7.71	124.36	118.29
3	A	1751	FMN	C4-C4A-C10	-7.46	115.01	119.95
2	B	1850	FAD	C4X-C4-N3	-6.83	114.09	123.43
2	A	1750	FAD	C4X-C4-N3	-6.75	114.20	123.43
3	B	1851	FMN	C4-C4A-C10	-6.49	115.66	119.95
3	B	1851	FMN	C4A-C4-N3	-5.39	116.06	123.43
2	A	1750	FAD	C10-C4X-N5	5.38	124.98	121.26
3	A	1751	FMN	C4A-C4-N3	-5.36	116.10	123.43
2	B	1850	FAD	C10-C4X-N5	5.36	124.96	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1851	FMN	C6-C5A-N5	-4.65	113.93	119.05
3	A	1751	FMN	C4A-N5-C5A	-4.08	112.70	116.77
3	B	1851	FMN	P-O5'-C5'	3.83	128.84	118.30
4	B	1852	NAP	PN-O3-PA	-3.65	120.31	132.83
4	B	1852	NAP	O7N-C7N-N7N	-3.63	117.43	122.58
3	B	1851	FMN	C4A-C10-N10	-3.62	116.58	120.30
4	A	1752	NAP	O7N-C7N-N7N	-3.56	117.53	122.58
3	B	1851	FMN	C9A-C5A-N5	3.51	127.85	122.36
2	A	1750	FAD	C1'-N10-C10	-3.49	115.28	118.41
3	A	1751	FMN	C6-C5A-N5	-3.47	115.23	119.05
2	B	1850	FAD	C5X-C9A-N10	-3.36	115.28	117.72
2	A	1750	FAD	C5X-C9A-N10	-3.35	115.29	117.72
3	A	1751	FMN	C4A-C10-N10	-3.32	116.89	120.30
2	A	1750	FAD	C4'-C3'-C2'	3.31	120.25	113.36
4	B	1852	NAP	C4A-C5A-N7A	3.20	112.74	109.40
2	B	1850	FAD	C4X-C10-N10	-3.19	117.03	120.30
4	A	1752	NAP	C3D-C2D-C1D	3.16	105.74	100.98
4	A	1752	NAP	C4A-C5A-N7A	3.14	112.67	109.40
2	B	1850	FAD	C1'-N10-C10	-3.07	115.66	118.41
3	A	1751	FMN	P-O5'-C5'	3.03	126.64	118.30
3	A	1751	FMN	C9A-C5A-N5	3.02	127.08	122.36
2	B	1850	FAD	C4'-C3'-C2'	3.01	119.62	113.36
3	A	1751	FMN	O4'-C4'-C3'	-3.01	101.78	109.10
3	A	1751	FMN	C1'-N10-C9A	3.00	120.65	118.29
2	A	1750	FAD	C1B-N9A-C4A	-3.00	121.37	126.64
3	B	1851	FMN	C4A-N5-C5A	-2.97	113.81	116.77
3	B	1851	FMN	O3P-P-O5'	-2.95	98.89	106.73
4	A	1752	NAP	PN-O3-PA	-2.94	122.73	132.83
3	A	1751	FMN	O3P-P-O5'	-2.93	98.93	106.73
2	A	1750	FAD	C4X-C10-N10	-2.88	117.34	120.30
4	B	1852	NAP	N3A-C2A-N1A	-2.87	124.19	128.68
3	A	1751	FMN	C4'-C3'-C2'	-2.80	107.54	113.36
4	A	1752	NAP	O7N-C7N-C3N	2.80	122.98	119.63
3	A	1751	FMN	O2P-P-O1P	2.78	121.56	110.68
4	B	1852	NAP	O7N-C7N-C3N	2.76	122.93	119.63
2	A	1750	FAD	C4-C4X-C10	-2.75	118.13	119.95
4	A	1752	NAP	N3A-C2A-N1A	-2.75	124.38	128.68
3	B	1851	FMN	C1'-N10-C9A	2.75	120.45	118.29
4	B	1852	NAP	C3D-C2D-C1D	2.75	105.11	100.98
4	B	1852	NAP	C6N-N1N-C2N	-2.74	119.47	121.97
3	B	1851	FMN	C5A-C9A-N10	-2.71	115.75	117.72
4	A	1752	NAP	C3N-C2N-N1N	2.69	123.06	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1852	NAP	C3N-C2N-N1N	2.65	123.02	120.43
4	A	1752	NAP	C6N-N1N-C2N	-2.65	119.56	121.97
2	B	1850	FAD	O2'-C2'-C1'	2.61	115.87	109.59
3	B	1851	FMN	O4'-C4'-C3'	-2.60	102.77	109.10
3	B	1851	FMN	C1'-N10-C10	2.59	120.73	118.41
3	B	1851	FMN	O2P-P-O1P	2.59	120.80	110.68
3	A	1751	FMN	C5A-C9A-N10	-2.45	115.94	117.72
2	B	1850	FAD	C9A-C5X-N5	2.45	126.20	122.36
2	B	1850	FAD	C6-C5X-N5	-2.45	116.35	119.05
2	B	1850	FAD	C1B-N9A-C4A	-2.38	122.46	126.64
2	A	1750	FAD	C9A-C5X-N5	2.37	126.07	122.36
3	B	1851	FMN	C9A-N10-C10	-2.37	118.81	121.91
2	B	1850	FAD	C4-C4X-C10	-2.32	118.41	119.95
2	A	1750	FAD	O2'-C2'-C1'	2.29	115.12	109.59
3	A	1751	FMN	C8M-C8-C7	2.29	125.44	120.74
2	B	1850	FAD	C4A-C5A-N7A	2.27	111.77	109.40
2	A	1750	FAD	C4A-C5A-N7A	2.25	111.75	109.40
2	A	1750	FAD	C6-C5X-N5	-2.20	116.62	119.05
2	A	1750	FAD	O3'-C3'-C4'	-2.14	103.63	108.81
4	B	1852	NAP	C2A-N1A-C6A	2.12	122.37	118.75
3	B	1851	FMN	C8M-C8-C7	2.07	124.99	120.74
2	B	1850	FAD	O3'-C3'-C4'	-2.07	103.82	108.81
4	A	1752	NAP	C2A-N1A-C6A	2.03	122.23	118.75

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1852	NAP	O4D-C4D-C5D-O5D
4	A	1752	NAP	O4D-C4D-C5D-O5D
4	B	1852	NAP	C3D-C4D-C5D-O5D
4	B	1852	NAP	C2B-O2B-P2B-O1X
2	A	1750	FAD	C3'-C4'-C5'-O5'
2	B	1850	FAD	C3'-C4'-C5'-O5'
2	A	1750	FAD	PA-O3P-P-O1P
4	A	1752	NAP	C3D-C4D-C5D-O5D
5	B	1753	EPE	C10-C9-N1-C2
2	B	1850	FAD	PA-O3P-P-O1P
4	A	1752	NAP	PA-O3-PN-O1N
4	A	1752	NAP	C2B-O2B-P2B-O1X
4	A	1752	NAP	C2B-O2B-P2B-O2X
4	A	1752	NAP	C2B-O2B-P2B-O3X

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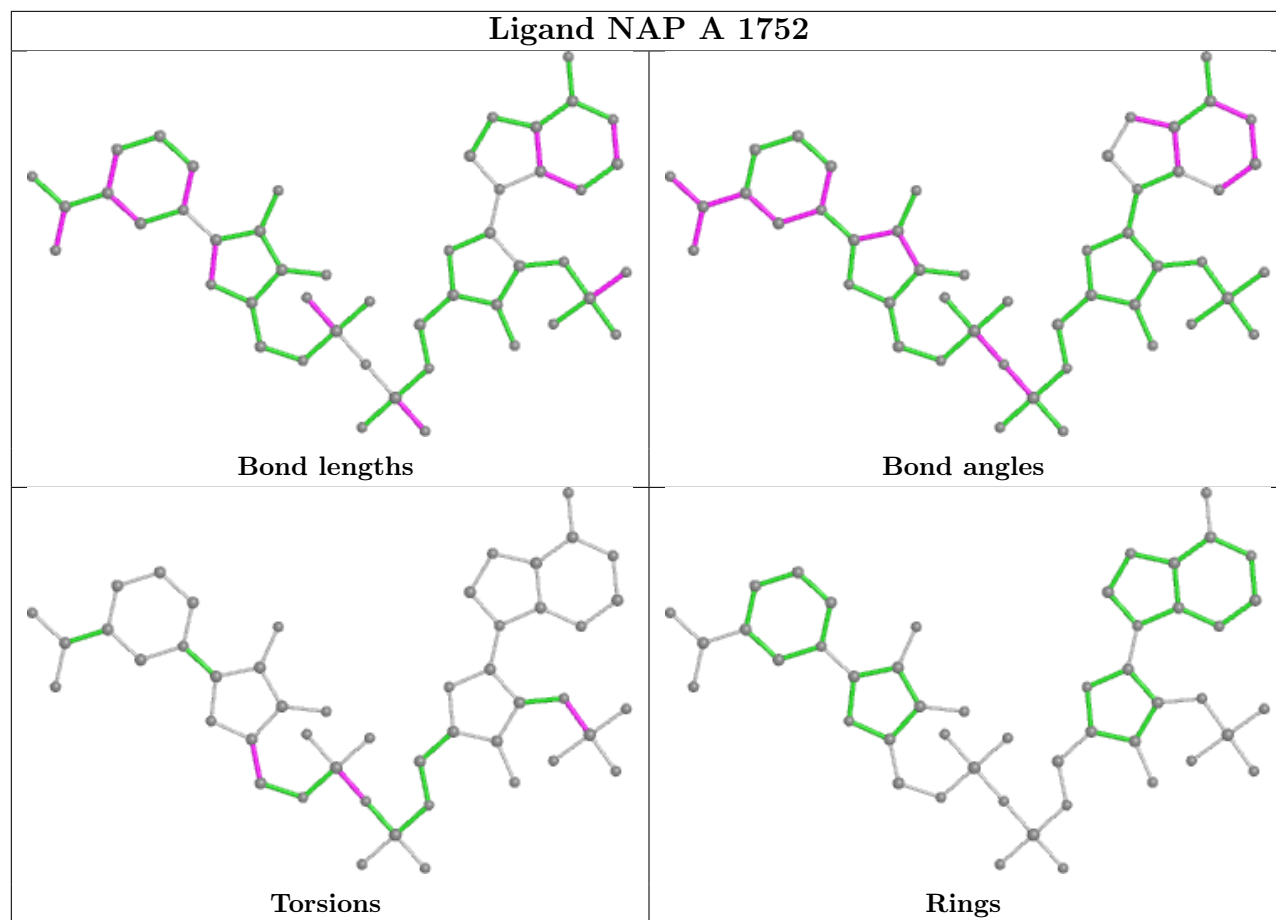
Mol	Chain	Res	Type	Atoms
2	A	1750	FAD	PA-O3P-P-O2P
2	B	1850	FAD	PA-O3P-P-O2P

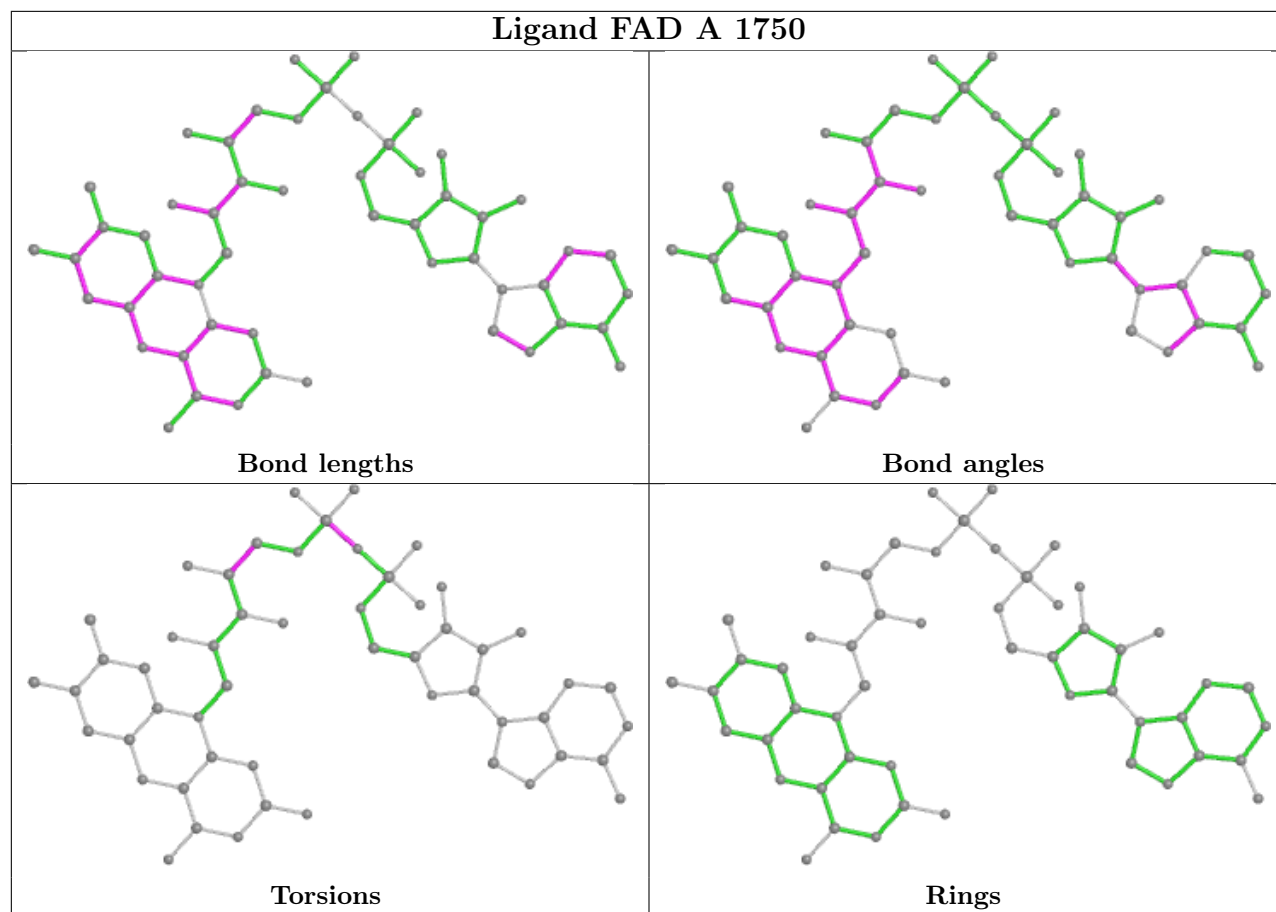
There are no ring outliers.

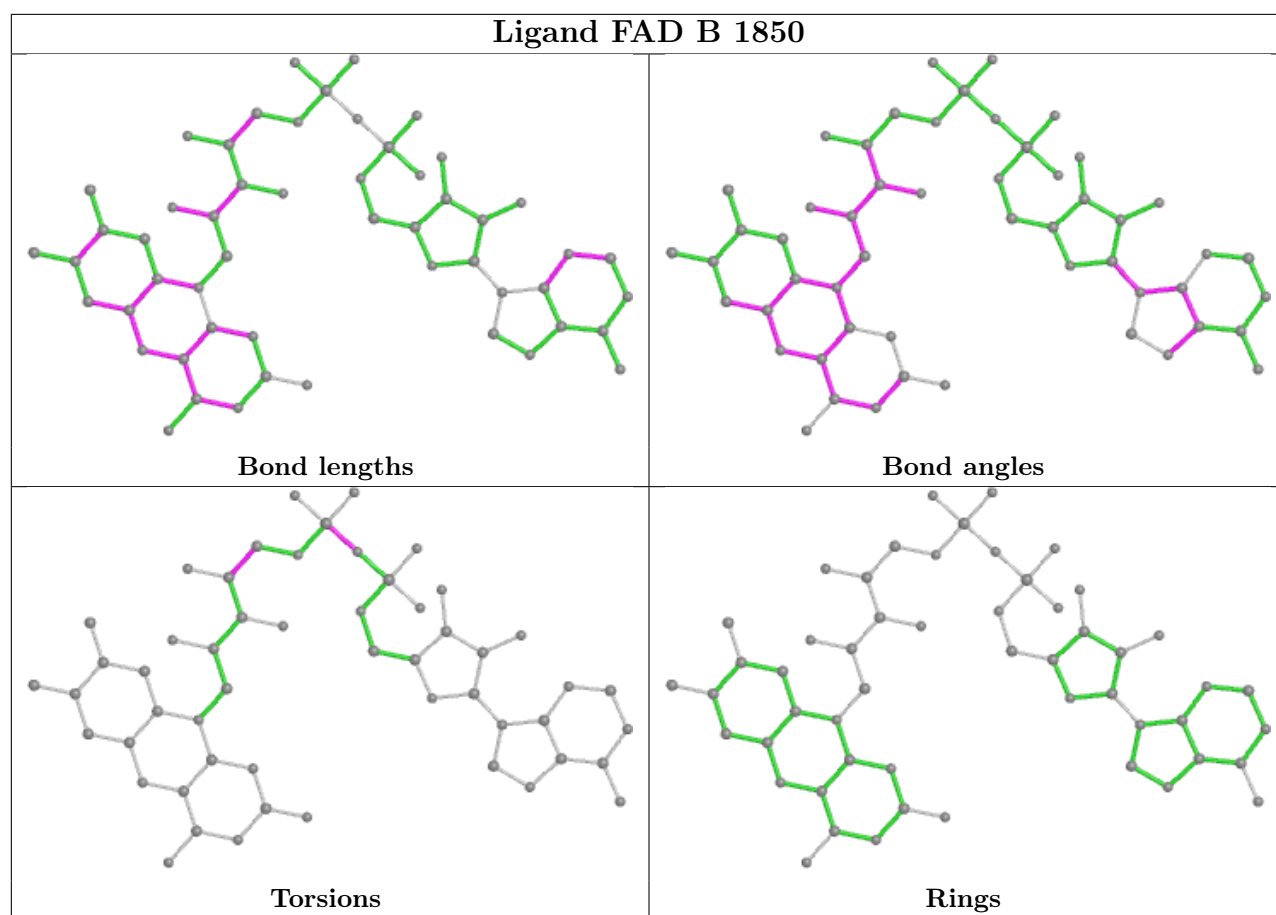
4 monomers are involved in 7 short contacts:

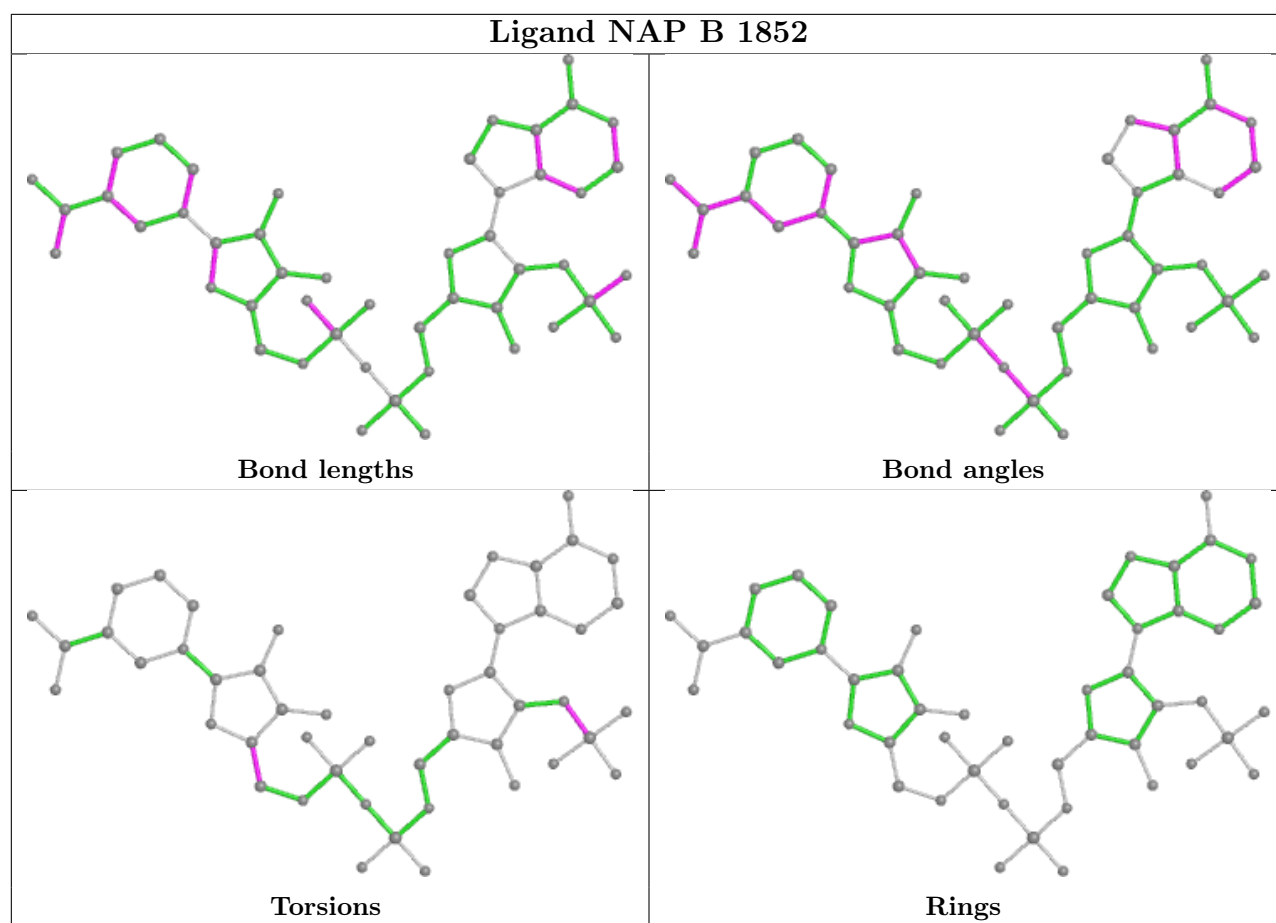
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1752	NAP	3	0
2	B	1850	FAD	1	0
4	B	1852	NAP	2	0
3	A	1751	FMN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

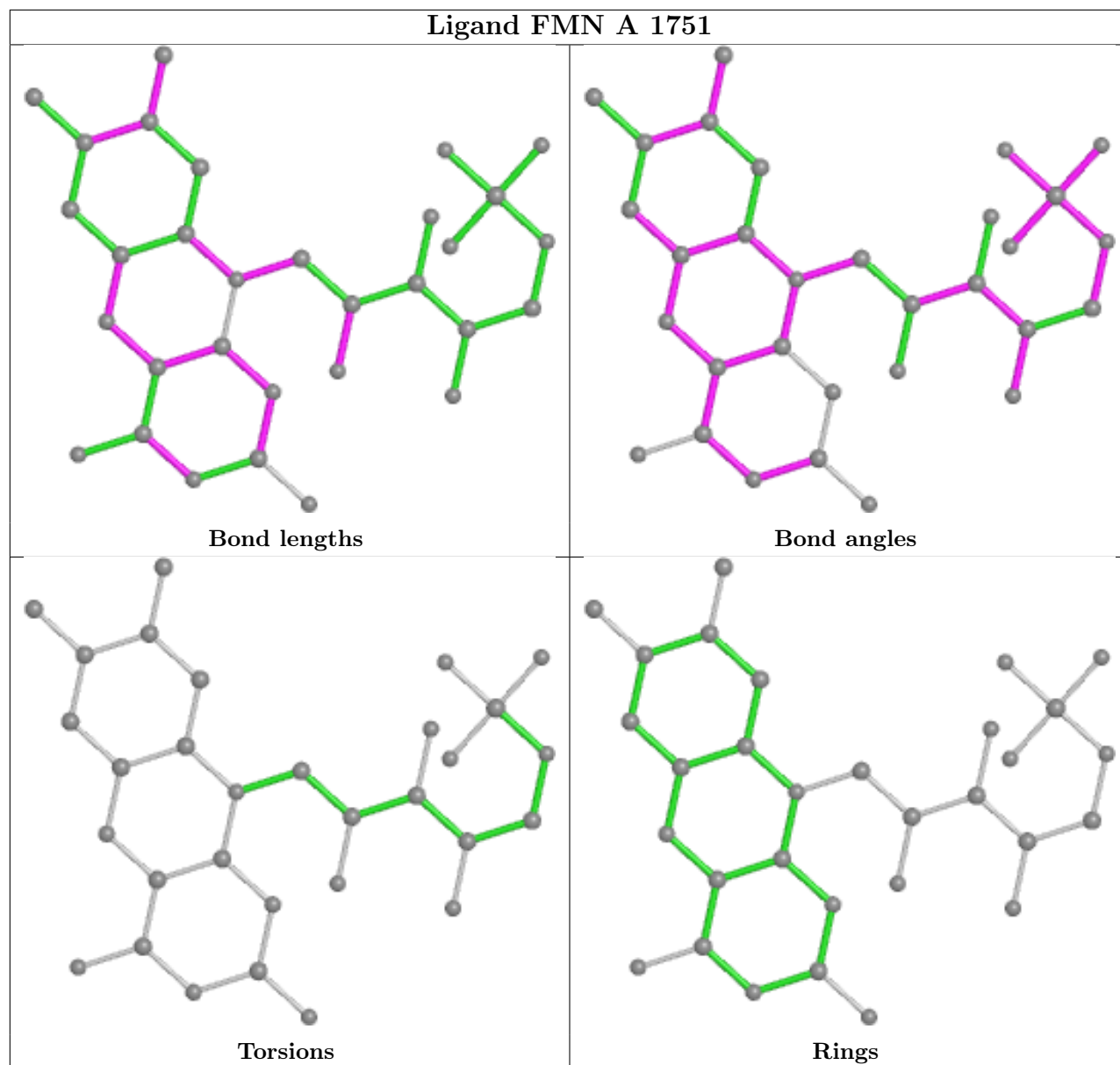


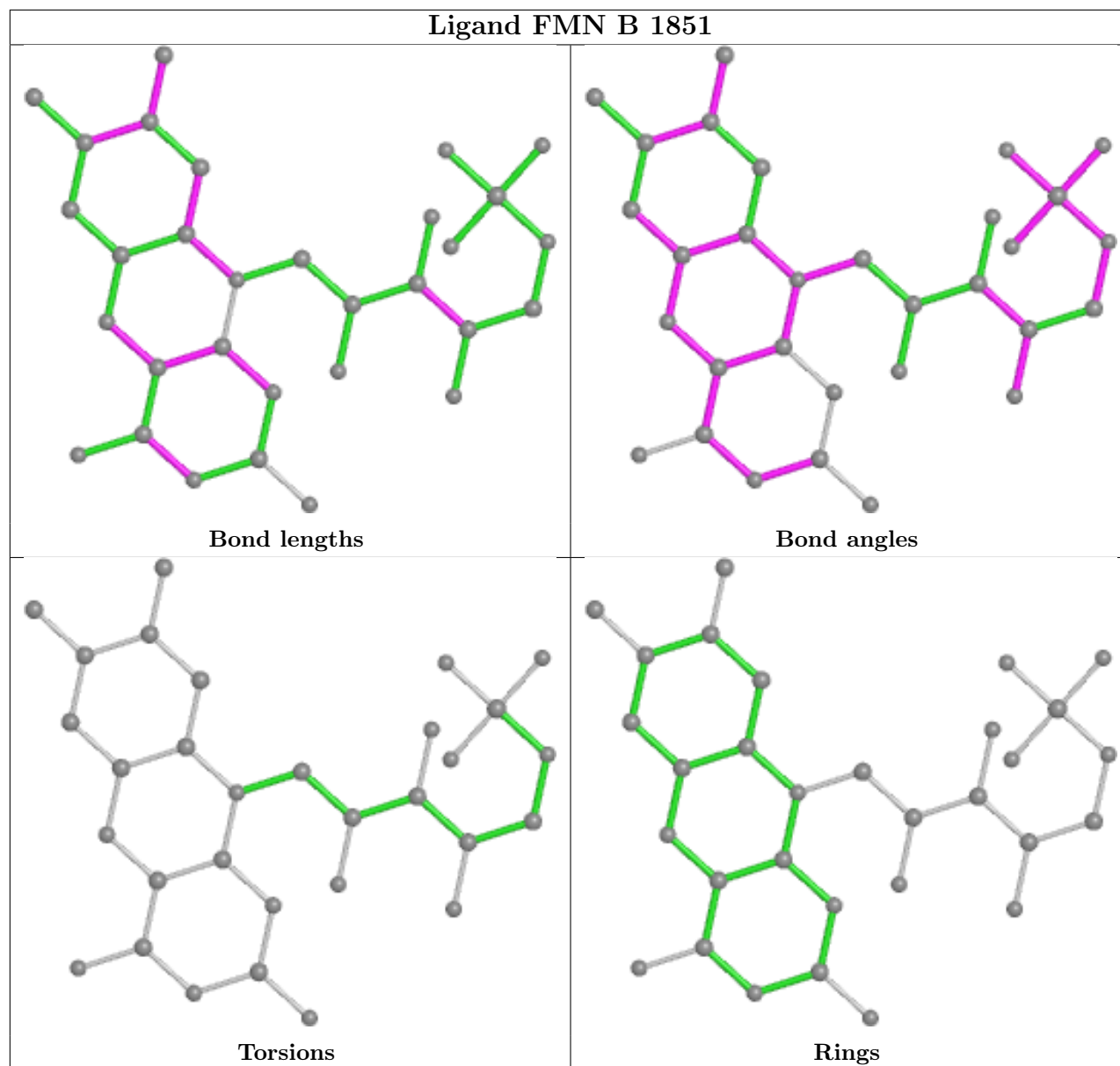






Ligand FMN A 1751





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	616/622 (99%)	0.05	27 (4%) 34 28	16, 26, 54, 100	0
1	B	614/622 (98%)	0.48	73 (11%) 4 3	13, 31, 81, 100	0
All	All	1230/1244 (98%)	0.26	100 (8%) 12 9	13, 28, 76, 100	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	500	ALA	14.9
1	A	503	ASN	11.4
1	A	501	GLY	10.6
1	B	502	GLU	10.2
1	B	501	GLY	9.5
1	B	237	GLY	8.9
1	B	241	SER	8.5
1	A	505	GLY	8.1
1	A	502	GLU	8.1
1	A	237	GLY	7.6
1	A	500	ALA	7.3
1	B	238	GLU	7.1
1	A	238	GLU	7.1
1	B	160	ASP	7.0
1	A	236	THR	6.7
1	B	233	VAL	6.5
1	B	240	SER	6.3
1	B	236	THR	6.3
1	A	504	GLY	6.2
1	B	503	ASN	6.1
1	A	175	ASN	5.9
1	B	158	GLU	5.8
1	A	506	ARG	5.7
1	B	504	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	140	TYR	5.3
1	B	505	GLY	5.0
1	B	239	GLU	5.0
1	A	174	GLY	4.9
1	B	128	ILE	4.9
1	A	180	HIS	4.6
1	B	159	THR	4.6
1	B	234	GLU	4.6
1	B	155	TRP	4.0
1	B	83	PHE	4.0
1	B	76	THR	4.0
1	B	163	LEU	4.0
1	B	98	LEU	3.8
1	B	120	ALA	3.8
1	B	82	VAL	3.8
1	B	95	ALA	3.6
1	B	132	LEU	3.5
1	B	252	ASP	3.5
1	B	254	ASP	3.5
1	B	104	ARG	3.4
1	B	192	LEU	3.4
1	B	75	LYS	3.3
1	B	187	TYR	3.3
1	B	176	LYS	3.3
1	B	161	VAL	3.2
1	B	142	GLU	3.2
1	B	253	MET	3.2
1	B	106	GLY	3.2
1	B	242	ILE	3.0
1	A	239	GLU	3.0
1	A	106	GLY	3.0
1	A	141	GLY	3.0
1	B	235	ALA	2.9
1	B	195	LEU	2.9
1	B	191	ARG	2.9
1	B	181	PHE	2.9
1	B	180	HIS	2.8
1	A	181	PHE	2.8
1	A	179	GLU	2.8
1	B	69	PHE	2.8
1	B	231	PHE	2.8
1	B	154	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	152	PHE	2.7
1	B	125	LEU	2.7
1	A	235	ALA	2.6
1	B	144	ASP	2.6
1	B	506	ARG	2.6
1	A	252	ASP	2.6
1	B	139	THR	2.6
1	A	273	LYS	2.6
1	B	150	GLN	2.5
1	A	234	GLU	2.5
1	B	129	ASP	2.4
1	B	147	ASP	2.4
1	A	160	ASP	2.4
1	B	255	VAL	2.4
1	B	130	LYS	2.4
1	B	80	ILE	2.4
1	B	140	TYR	2.3
1	B	94	PHE	2.3
1	A	178	TYR	2.3
1	B	78	ARG	2.3
1	B	197	ALA	2.2
1	B	162	ASP	2.2
1	B	103	HIS	2.2
1	A	158	GLU	2.2
1	B	156	LEU	2.2
1	B	141	GLY	2.2
1	B	229	GLU	2.2
1	B	169	ALA	2.1
1	B	164	THR	2.1
1	A	63	PRO	2.1
1	B	77	GLY	2.1
1	B	123	SER	2.0
1	B	166	VAL	2.0
1	B	210	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

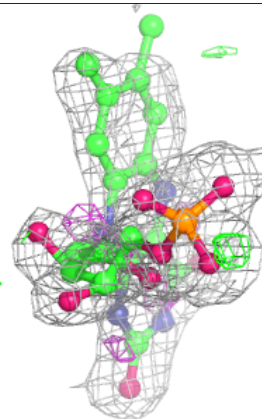
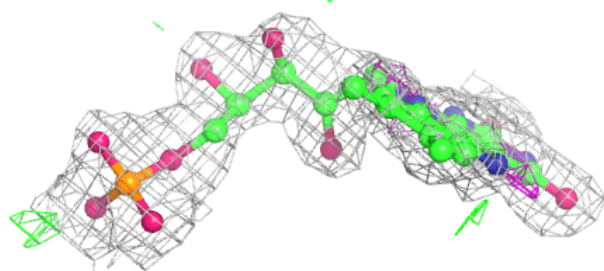
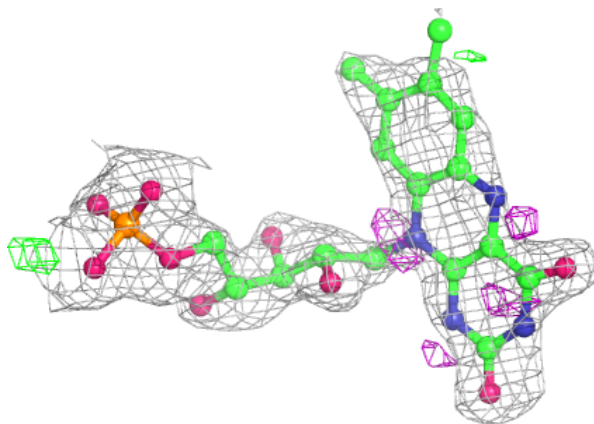
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EPE	B	1753	15/15	0.85	0.22	46,52,65,69	0
3	FMN	B	1851	31/31	0.86	0.23	39,48,51,54	0
3	FMN	A	1751	31/31	0.92	0.15	24,38,47,49	0
4	NAP	B	1852	48/48	0.95	0.14	14,22,87,88	0
4	NAP	A	1752	48/48	0.96	0.11	17,23,79,84	0
2	FAD	B	1850	53/53	0.97	0.09	14,19,30,34	0
2	FAD	A	1750	53/53	0.97	0.10	14,19,33,41	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.

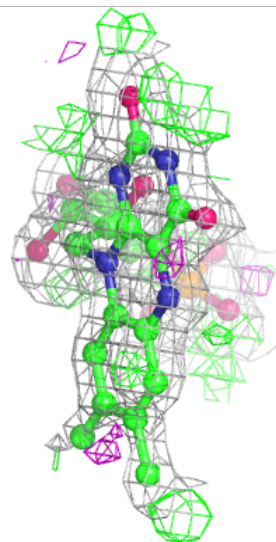
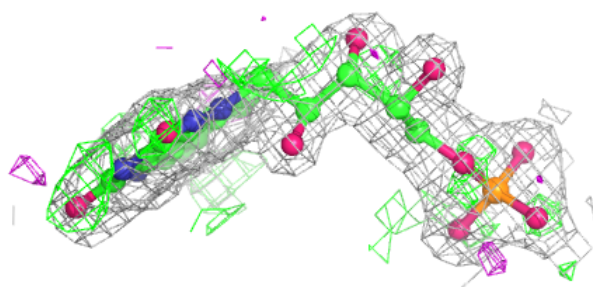
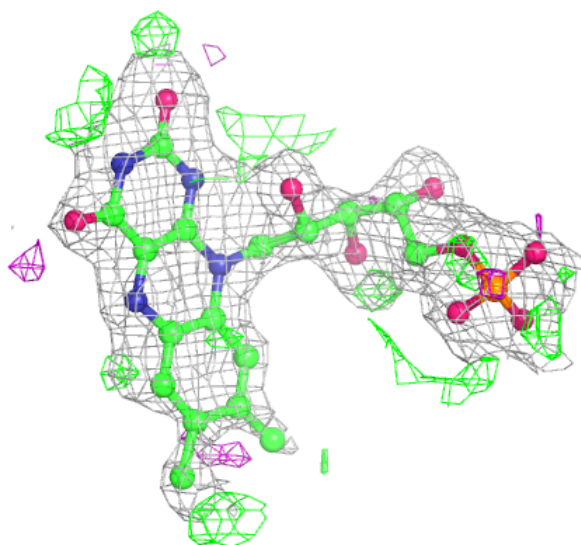
Electron density around FMN B 1851:

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



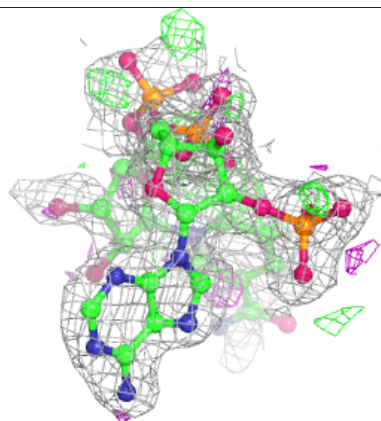
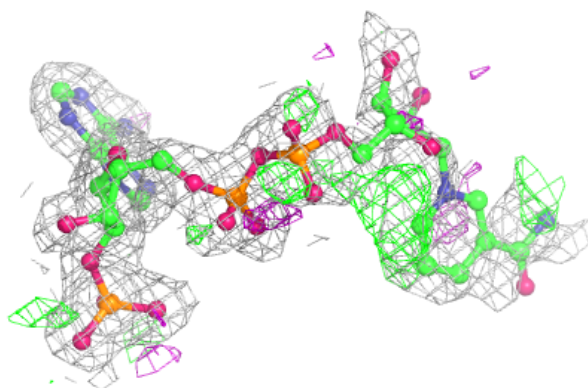
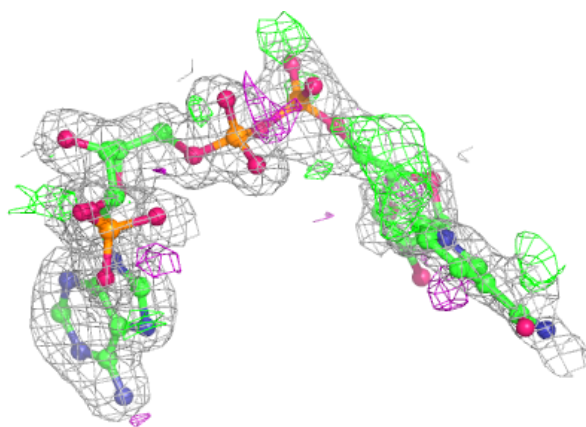
Electron density around FMN A 1751:

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



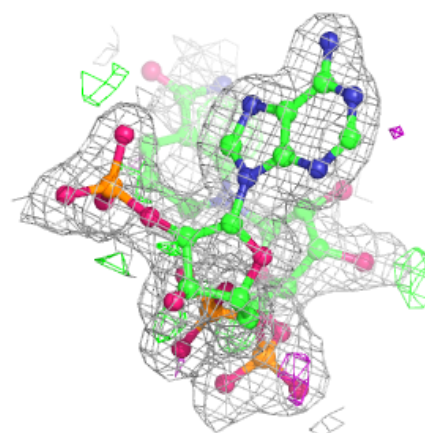
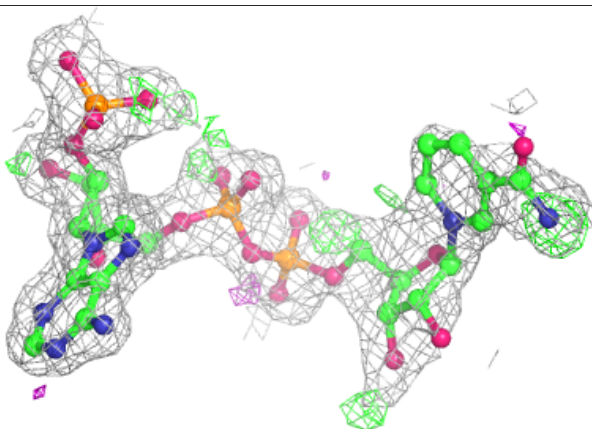
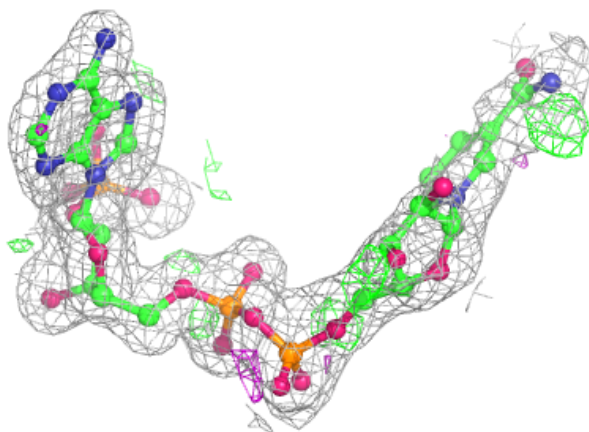
Electron density around NAP B 1852:

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

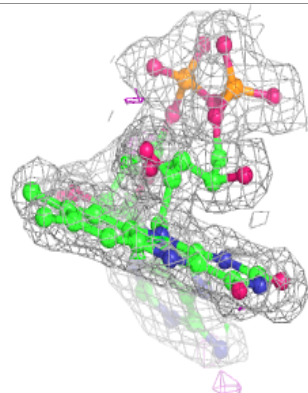
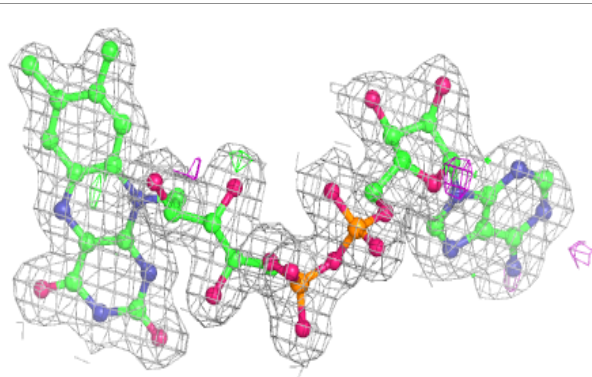
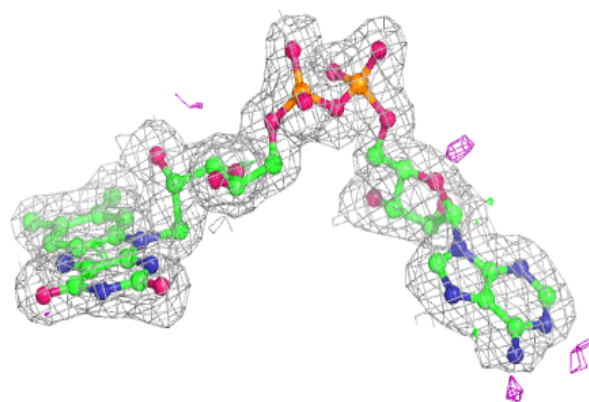


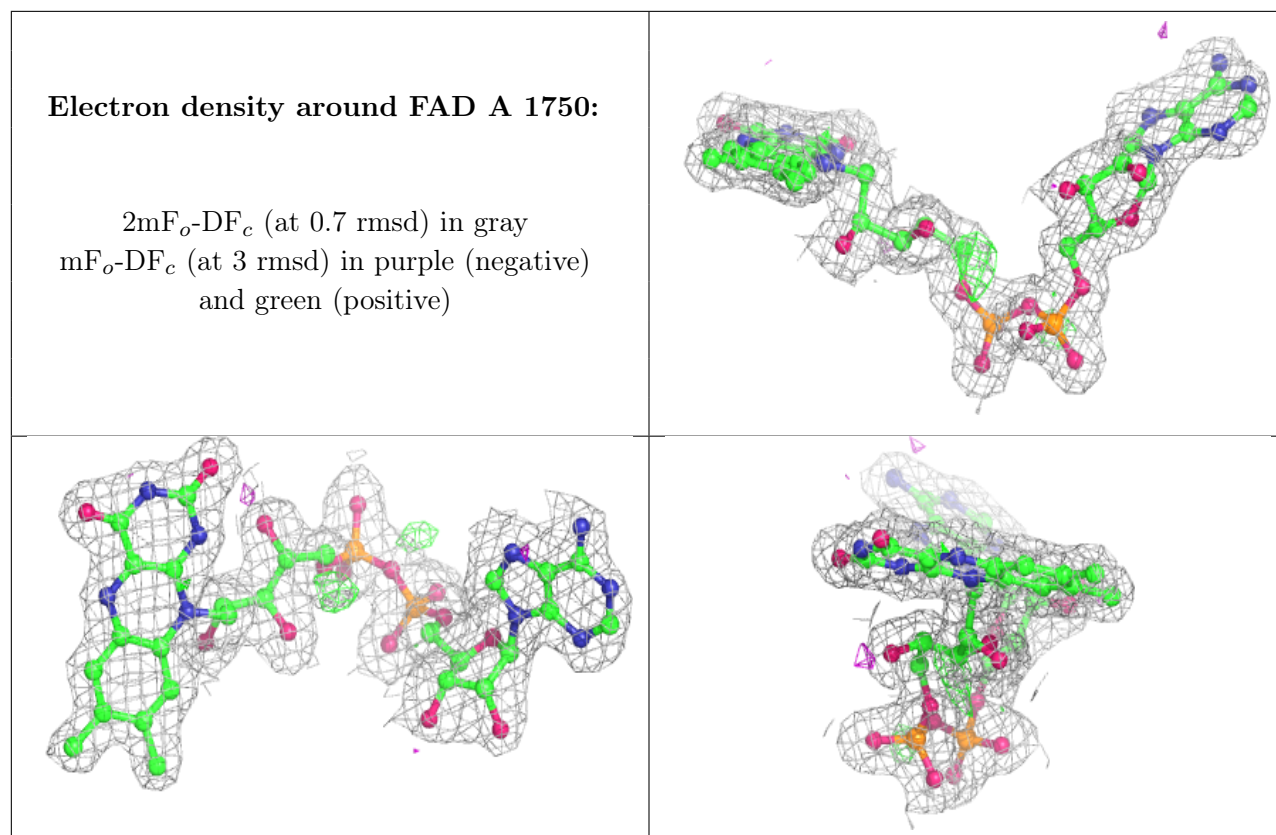
Electron density around NAP A 1752:

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

**Electron density around FAD B 1850:**

$2mF_o-DF_c$ (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.