



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:57 AM UTC

PDB ID : 3QFR / pdb_00003qfr
Title : Crystal Structure of Human NADPH-Cytochrome P450 Reductase (R457H Mutant)
Authors : Xia, C.; Marohnic, C.; Panda, S.P.; Masters, B.S.; Kim, J.-J.P.
Deposited on : 2011-01-22
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

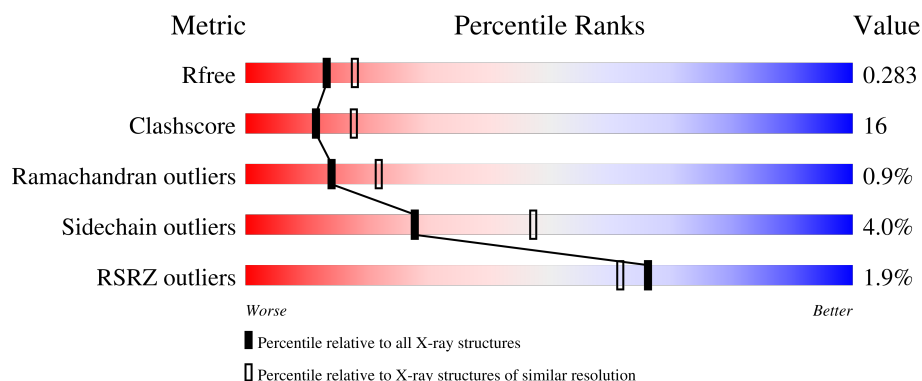
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	618	% 69% 26% ..
1	B	618	3% 60% 33% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9964 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	604	Total	C	N	O	S	0	0	0
			4813	3047	833	910	23			
1	B	603	Total	C	N	O	S	0	0	0
			4820	3049	835	913	23			

There are 10 discrepancies between the modelled and reference sequences:

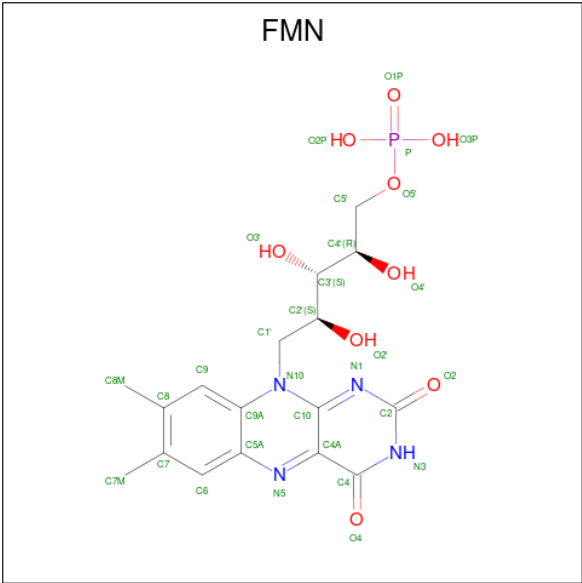
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP P16435
A	64	SER	-	expression tag	UNP P16435
A	65	HIS	-	expression tag	UNP P16435
A	66	MET	-	expression tag	UNP P16435
A	457	HIS	ARG	engineered mutation	UNP P16435
B	63	GLY	-	expression tag	UNP P16435
B	64	SER	-	expression tag	UNP P16435
B	65	HIS	-	expression tag	UNP P16435
B	66	MET	-	expression tag	UNP P16435
B	457	HIS	ARG	engineered mutation	UNP P16435

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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 (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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		

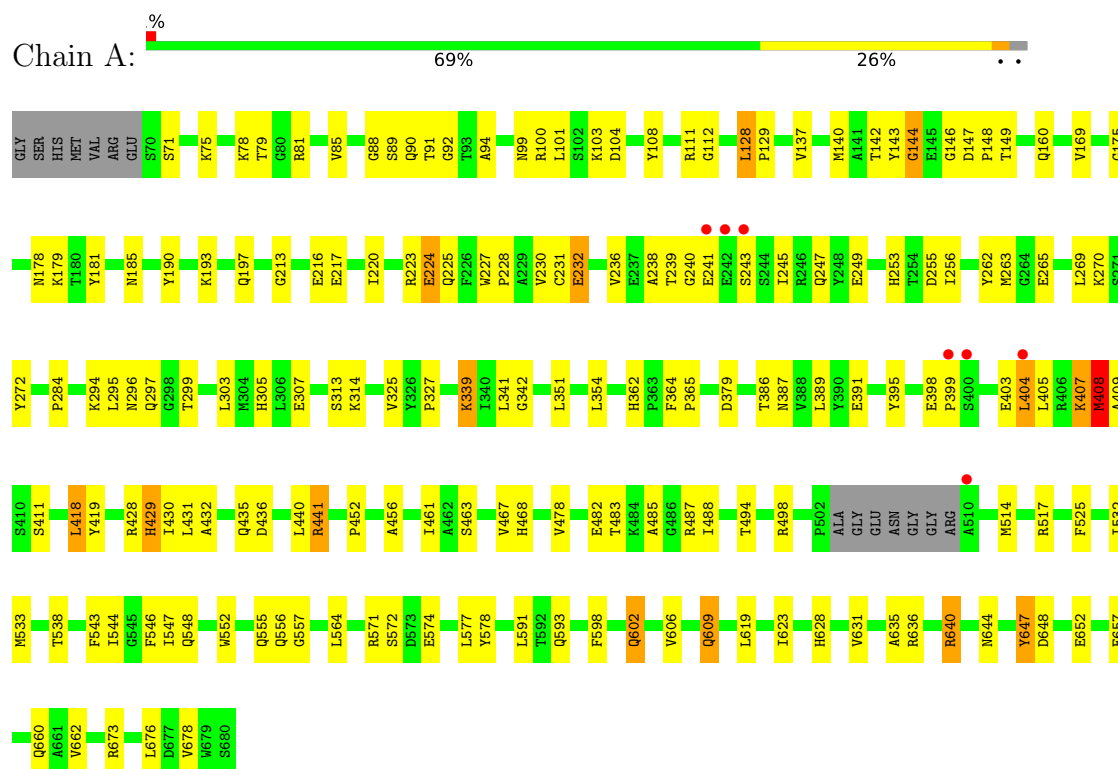
- # NAP

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	72	Total O 72 72	0	0
6	B	28	Total O 28 28	0	0

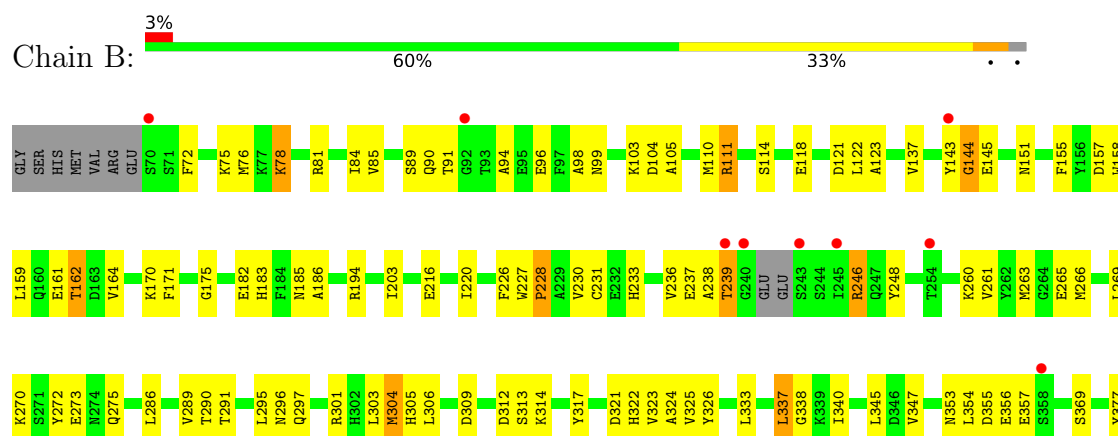
3 Residue-property plots

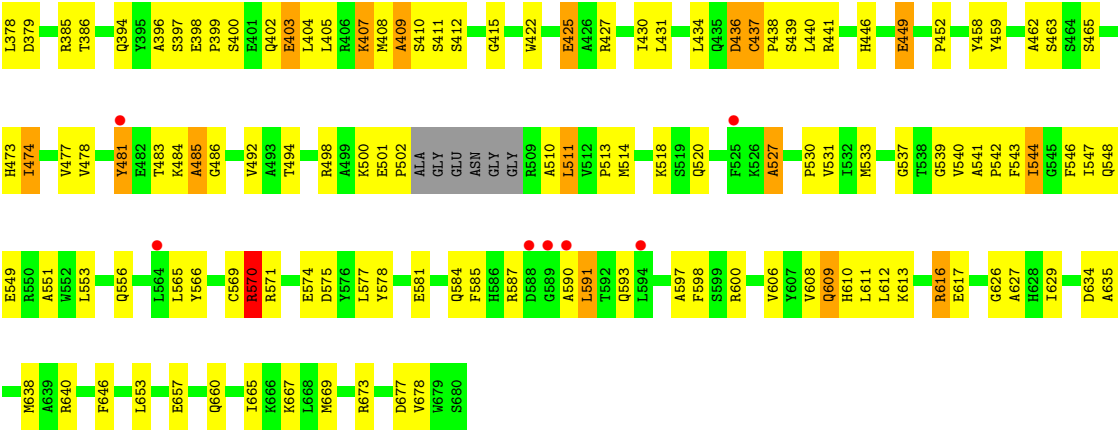
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	70.28Å 120.39Å 156.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.72 – 2.40 45.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.4 (45.72-2.40) 90.4 (45.72-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.285 0.227 , 0.283	Depositor DCC
R_{free} test set	2384 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 19.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9964	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% 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: FMN, FAD, CA, NAP

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	0.49	0/4924	0.94	13/6667 (0.2%)
1	B	0.44	0/4930	0.95	17/6671 (0.3%)
All	All	0.46	0/9854	0.94	30/13338 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	TYR	N-CA-C	7.35	122.54	113.50
1	A	92	GLY	N-CA-C	7.05	125.45	115.30
1	B	492	VAL	N-CA-C	7.02	117.73	110.36
1	B	612	LEU	N-CA-C	-6.98	104.75	113.55
1	A	88	GLY	N-CA-C	-6.00	98.96	113.18
1	A	662	VAL	N-CA-C	-5.95	104.55	110.62
1	B	544	ILE	N-CA-C	-5.91	103.71	111.09
1	B	261	VAL	N-CA-C	5.91	117.09	108.53
1	B	437	CYS	CA-C-N	5.90	127.22	119.84
1	B	437	CYS	C-N-CA	5.90	127.22	119.84
1	A	636	ARG	N-CA-C	5.63	117.11	110.97
1	B	378	LEU	N-CA-C	5.63	118.73	109.72
1	A	514	MET	N-CA-C	5.52	116.65	108.86
1	B	570	ARG	N-CA-C	5.49	117.70	111.11
1	B	171	PHE	N-CA-C	5.45	117.26	109.14
1	A	140	MET	N-CA-C	5.40	117.76	109.07
1	A	149	THR	N-CA-C	-5.38	103.38	110.43
1	A	647	TYR	N-CA-C	-5.36	105.08	111.03
1	B	610	HIS	N-CA-C	-5.33	105.91	112.90
1	A	213	GLY	N-CA-C	-5.32	100.58	113.18
1	A	398	GLU	CA-C-N	5.28	124.73	119.24
1	A	398	GLU	C-N-CA	5.28	124.73	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	ALA	N-CA-C	-5.27	106.87	113.72
1	A	71	SER	N-CA-C	-5.25	100.74	109.46
1	B	182	GLU	N-CA-C	5.23	116.67	111.07
1	B	449	GLU	N-CA-C	-5.17	107.10	113.41
1	B	474	ILE	N-CA-C	5.16	115.91	108.48
1	A	456	ALA	N-CA-C	-5.16	103.23	110.50
1	B	422	TRP	N-CA-C	5.14	116.96	111.36
1	B	304	MET	N-CA-C	5.05	117.36	109.52

There are no chirality outliers.

There are no planarity outliers.

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	4813	0	4666	124	0
1	B	4820	0	4684	186	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	31	0	19	0	0
3	B	31	0	19	1	0
4	A	31	0	11	2	0
4	B	31	0	11	1	0
5	A	1	0	0	0	0
6	A	72	0	0	6	0
6	B	28	0	0	6	0
All	All	9964	0	9472	310	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 16.

All (310) 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:A:441:ARG:HH11	1:A:441:ARG:HB3	1.20	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:MET:HE2	1:B:306:LEU:HD11	1.44	0.99
1:B:275:GLN:HE22	1:B:286:LEU:H	1.12	0.97
1:A:657:GLU:H	1:A:660:GLN:HE21	1.11	0.93
1:B:379:ASP:HB3	1:B:452:PRO:HG2	1.52	0.89
1:A:99:ASN:HB3	6:A:21:HOH:O	1.74	0.88
1:B:609:GLN:H	1:B:609:GLN:HE21	1.24	0.85
1:B:353:ASN:HD22	1:B:354:LEU:N	1.74	0.85
1:A:609:GLN:HE22	4:A:753:NAP:H2A	1.41	0.84
1:B:530:PRO:HG2	1:B:627:ALA:HB2	1.59	0.83
1:B:304:MET:HE1	1:B:498:ARG:HA	1.65	0.79
1:B:609:GLN:HE22	4:B:753:NAP:H2A	1.48	0.78
1:A:305:HIS:HD2	1:A:578:TYR:OH	1.68	0.77
1:B:597:ALA:HB2	1:B:611:LEU:HD22	1.67	0.76
1:B:220:ILE:CG2	1:B:411:SER:HB3	2.18	0.74
1:B:305:HIS:HD2	1:B:578:TYR:OH	1.70	0.74
1:B:353:ASN:ND2	1:B:355:ASP:H	1.86	0.73
1:A:657:GLU:H	1:A:660:GLN:NE2	1.85	0.73
1:B:144:GLY:O	1:B:145:GLU:HG2	1.89	0.73
1:A:429:HIS:HD2	1:A:432:ALA:H	1.37	0.72
1:A:89:SER:HB2	1:A:94:ALA:HB3	1.69	0.72
1:A:249:GLU:HB2	1:A:354:LEU:HD21	1.72	0.72
1:A:160:GLN:HG2	1:A:190:TYR:OH	1.89	0.71
1:A:441:ARG:HB3	1:A:441:ARG:NH1	2.01	0.71
1:B:597:ALA:HB1	1:B:606:VAL:HG12	1.72	0.71
1:B:220:ILE:HG22	1:B:411:SER:HB3	1.72	0.70
1:B:321:ASP:OD1	1:B:518:LYS:HA	1.91	0.70
1:B:404:LEU:HD23	1:B:408:MET:HE2	1.74	0.70
1:B:609:GLN:H	1:B:609:GLN:NE2	1.90	0.70
1:B:569:CYS:O	1:B:598:PHE:HA	1.92	0.69
1:B:158:TRP:O	1:B:162:THR:HG22	1.95	0.67
1:B:386:THR:HB	1:B:409:ALA:HA	1.76	0.67
1:B:275:GLN:NE2	1:B:286:LEU:H	1.90	0.67
1:A:543:PHE:O	1:A:547:ILE:HG12	1.95	0.67
1:A:544:ILE:O	1:A:548:GLN:HG3	1.94	0.67
1:B:353:ASN:HD22	1:B:354:LEU:H	1.44	0.66
1:A:225:GLN:HG3	6:A:40:HOH:O	1.94	0.66
1:B:81:ARG:HH11	1:B:81:ARG:HG3	1.61	0.66
1:B:396:ALA:HB3	1:B:402:GLN:HG2	1.77	0.65
1:B:397:SER:HB2	1:B:439:SER:HB2	1.78	0.65
1:A:609:GLN:H	1:A:609:GLN:NE2	1.95	0.64
1:B:265:GLU:HA	1:B:272:TYR:CE1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LYS:NZ	1:B:233:HIS:HE1	1.95	0.64
1:B:544:ILE:O	1:B:548:GLN:HG3	1.98	0.64
1:B:338:GLY:HA3	1:B:345:LEU:HD11	1.78	0.63
1:B:75:LYS:HE2	1:B:357:GLU:O	1.98	0.63
1:A:297:GLN:HA	1:A:297:GLN:NE2	2.14	0.63
1:A:147:ASP:HB3	1:A:148:PRO:HD2	1.81	0.63
1:B:584:GLN:NE2	1:B:587:ARG:NH1	2.47	0.62
1:A:379:ASP:HB3	1:A:452:PRO:HG2	1.81	0.62
1:B:591:LEU:HD22	1:B:593:GLN:O	2.00	0.62
1:A:485:ALA:HB1	1:A:487:ARG:NH2	2.16	0.61
1:B:626:GLY:HA2	1:B:673:ARG:NH2	2.15	0.61
1:A:429:HIS:CD2	1:A:432:ALA:H	2.18	0.61
1:B:286:LEU:CD2	1:B:513:PRO:HG3	2.30	0.61
1:A:313:SER:O	1:A:314:LYS:HB2	1.98	0.61
1:A:303:LEU:HD22	1:A:577:LEU:HD21	1.83	0.60
1:A:657:GLU:N	1:A:660:GLN:HE21	1.92	0.60
1:B:286:LEU:HD22	1:B:511:LEU:HB3	1.82	0.60
1:B:110:MET:HE2	1:B:236:VAL:HG21	1.82	0.60
1:B:145:GLU:C	1:B:183:HIS:HD2	2.09	0.60
1:B:246:ARG:NH1	1:B:449:GLU:OE2	2.33	0.60
1:A:657:GLU:HB2	1:A:660:GLN:HG3	1.83	0.60
1:A:299:THR:HG22	6:A:685:HOH:O	2.01	0.60
1:B:400:SER:HA	1:B:403:GLU:OE2	2.01	0.60
1:A:609:GLN:H	1:A:609:GLN:HE21	1.50	0.60
1:B:122:LEU:HG	1:B:155:PHE:CD1	2.37	0.60
1:B:613:LYS:O	1:B:616:ARG:HG3	2.02	0.60
1:A:435:GLN:HE21	1:A:487:ARG:HH11	1.50	0.59
1:A:399:PRO:O	1:A:403:GLU:HG2	2.03	0.59
1:B:355:ASP:O	1:B:357:GLU:N	2.35	0.59
1:B:323:VAL:HG13	1:B:459:TYR:HB2	1.84	0.59
1:B:410:SER:HB3	6:B:684:HOH:O	2.01	0.59
1:B:333:LEU:HD12	1:B:431:LEU:HD22	1.85	0.58
1:B:396:ALA:HB3	1:B:402:GLN:CG	2.33	0.58
1:A:405:LEU:HD11	1:A:440:LEU:HD22	1.86	0.58
1:A:104:ASP:OD1	1:A:223:ARG:HD2	2.04	0.57
1:A:482:GLU:HG3	1:A:488:ILE:HD13	1.86	0.57
1:B:99:ASN:ND2	1:B:114:SER:CB	2.66	0.57
1:B:570:ARG:C	1:B:571:ARG:HG3	2.30	0.57
1:A:404:LEU:HD22	1:A:418:LEU:HD11	1.87	0.57
1:A:297:GLN:HA	1:A:297:GLN:HE21	1.69	0.57
1:A:339:LYS:NZ	1:A:339:LYS:HB3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:VAL:HG12	1:B:514:MET:HB3	1.87	0.56
1:B:226:PHE:O	1:B:230:VAL:HG23	2.06	0.56
1:B:227:TRP:HB2	1:B:228:PRO:HD3	1.87	0.56
1:A:81:ARG:NH1	1:A:112:GLY:O	2.38	0.56
1:A:238:ALA:C	1:A:240:GLY:H	2.13	0.56
1:A:305:HIS:CD2	1:A:578:TYR:OH	2.56	0.56
1:B:584:GLN:NE2	1:B:587:ARG:HH12	2.03	0.55
1:B:657:GLU:H	1:B:660:GLN:NE2	2.04	0.55
1:B:379:ASP:CB	1:B:452:PRO:HG2	2.32	0.55
1:A:227:TRP:HB2	1:A:228:PRO:HD3	1.89	0.55
1:B:289:VAL:HG23	1:B:510:ALA:O	2.07	0.55
1:A:295:LEU:HD11	1:A:305:HIS:HB2	1.88	0.55
1:A:407:LYS:NZ	1:A:407:LYS:HB3	2.22	0.55
1:B:170:LYS:HZ3	1:B:233:HIS:HE1	1.53	0.55
1:A:552:TRP:O	1:A:556:GLN:HG2	2.07	0.55
1:B:78:LYS:HB2	1:B:78:LYS:NZ	2.22	0.54
1:A:224:GLU:CD	1:A:411:SER:HB2	2.32	0.54
1:B:296:ASN:HB2	1:B:574:GLU:O	2.08	0.54
1:B:616:ARG:HB3	1:B:653:LEU:HD21	1.90	0.54
1:B:324:ALA:HB2	1:B:458:TYR:CD1	2.43	0.54
1:A:571:ARG:HD3	1:A:574:GLU:OE2	2.08	0.54
1:B:404:LEU:O	1:B:407:LYS:HG2	2.07	0.54
1:A:231:CYS:HA	1:A:236:VAL:HG23	1.90	0.54
1:B:118:GLU:HB2	1:B:151:ASN:O	2.08	0.54
1:A:628:HIS:CE1	1:A:673:ARG:HG2	2.43	0.53
1:B:322:HIS:HE1	1:B:677:ASP:OD1	1.91	0.53
1:B:570:ARG:HG2	1:B:600:ARG:HD2	1.91	0.53
1:B:609:GLN:HE21	1:B:609:GLN:N	2.01	0.53
1:B:353:ASN:HD22	1:B:353:ASN:C	2.15	0.53
1:B:543:PHE:O	1:B:547:ILE:HG13	2.08	0.53
1:A:387:ASN:O	1:A:391:GLU:HG2	2.09	0.53
1:A:631:VAL:HB	1:A:676:LEU:HD23	1.91	0.53
1:B:286:LEU:HD23	1:B:513:PRO:HG3	1.91	0.53
1:B:99:ASN:O	1:B:103:LYS:HG3	2.08	0.53
1:B:478:VAL:HA	1:B:494:THR:HB	1.90	0.53
1:B:549:GLU:O	1:B:553:LEU:HG	2.08	0.52
1:B:175:GLY:C	1:B:185:ASN:HD21	2.18	0.52
1:B:425:GLU:HG2	1:B:484:LYS:HZ2	1.75	0.52
1:B:313:SER:O	1:B:314:LYS:HB2	2.09	0.52
1:A:85:VAL:HA	1:A:137:VAL:O	2.09	0.52
1:B:398:GLU:H	1:B:439:SER:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HE2	1:A:247:GLN:NE2	2.25	0.52
1:A:483:THR:HB	6:A:18:HOH:O	2.10	0.52
1:B:530:PRO:HG2	1:B:627:ALA:CB	2.36	0.51
1:B:635:ALA:HB2	1:B:678:VAL:HB	1.92	0.51
1:B:90:GLN:HB3	1:B:143:TYR:CZ	2.45	0.51
1:B:404:LEU:CD2	1:B:408:MET:HE2	2.40	0.51
1:A:193:LYS:O	1:A:197:GLN:HG3	2.10	0.51
1:A:428:ARG:NE	1:A:436:ASP:OD1	2.40	0.51
1:B:286:LEU:HD21	1:B:513:PRO:HG3	1.92	0.51
1:B:547:ILE:HD11	1:B:565:LEU:HD22	1.92	0.51
1:B:415:GLY:HA3	6:B:684:HOH:O	2.10	0.51
1:B:437:CYS:N	1:B:438:PRO:HD3	2.26	0.50
1:B:295:LEU:HD21	1:B:305:HIS:HB2	1.93	0.50
1:B:405:LEU:HD23	1:B:408:MET:CE	2.41	0.50
1:A:262:TYR:O	1:A:263:MET:HE2	2.12	0.50
1:A:609:GLN:HE21	1:A:609:GLN:N	2.10	0.50
1:B:462:ALA:HA	1:B:541:ALA:O	2.12	0.50
1:A:341:LEU:O	1:A:342:GLY:C	2.54	0.50
1:B:89:SER:HB2	1:B:94:ALA:HB3	1.94	0.50
1:B:483:THR:OG1	1:B:484:LYS:N	2.44	0.50
1:B:303:LEU:HD22	1:B:577:LEU:HD21	1.93	0.50
1:B:398:GLU:H	1:B:439:SER:CB	2.25	0.50
1:A:619:LEU:O	1:A:623:ILE:HG13	2.12	0.49
1:B:286:LEU:HD13	1:B:511:LEU:HD23	1.93	0.49
1:A:297:GLN:HE21	1:A:297:GLN:CA	2.24	0.49
1:A:564:LEU:HD23	1:A:593:GLN:NE2	2.27	0.49
1:A:243:SER:O	1:A:245:ILE:HG13	2.13	0.49
1:A:478:VAL:HA	1:A:494:THR:HB	1.93	0.49
1:B:657:GLU:H	1:B:660:GLN:HE21	1.61	0.49
1:A:108:TYR:CD1	1:A:231:CYS:SG	3.05	0.49
1:A:407:LYS:O	1:A:409:ALA:N	2.46	0.49
1:A:478:VAL:HG21	1:A:498:ARG:HD2	1.95	0.49
1:B:266:MET:HE3	1:B:326:TYR:CD2	2.47	0.49
1:B:481:TYR:CD1	1:B:481:TYR:N	2.81	0.49
1:A:253:HIS:CD2	1:A:256:ILE:HD12	2.48	0.49
1:B:337:LEU:HG	1:B:431:LEU:HD13	1.95	0.49
1:B:581:GLU:O	1:B:585:PHE:CD2	2.66	0.49
1:A:100:ARG:CZ	1:A:387:ASN:HD22	2.26	0.49
1:B:90:GLN:HB3	1:B:143:TYR:OH	2.13	0.49
1:B:500:LYS:HD3	1:B:510:ALA:HB1	1.94	0.49
1:A:238:ALA:C	1:A:240:GLY:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:MET:HE1	1:A:547:ILE:CD1	2.43	0.48
1:B:340:ILE:HD11	1:B:434:LEU:O	2.12	0.48
1:B:483:THR:HG21	6:B:52:HOH:O	2.12	0.48
1:A:91:THR:HG23	1:A:143:TYR:OH	2.13	0.48
1:A:75:LYS:HA	1:A:78:LYS:HG2	1.96	0.48
1:A:351:LEU:O	1:A:362:HIS:HD2	1.97	0.48
1:B:570:ARG:O	1:B:571:ARG:HG3	2.12	0.48
1:B:581:GLU:N	1:B:581:GLU:OE1	2.44	0.48
1:A:79:THR:OG1	1:A:81:ARG:HG2	2.14	0.48
1:A:104:ASP:HB2	1:A:227:TRP:CZ2	2.48	0.48
1:A:441:ARG:HH11	1:A:441:ARG:CB	2.07	0.48
1:B:183:HIS:HB3	1:B:186:ALA:HB2	1.95	0.48
1:B:304:MET:CE	1:B:306:LEU:HD11	2.31	0.47
1:B:485:ALA:HB3	6:B:52:HOH:O	2.13	0.47
1:B:263:MET:N	1:B:265:GLU:OE1	2.34	0.47
1:A:430:ILE:HG23	1:A:431:LEU:N	2.29	0.47
1:B:477:VAL:O	1:B:477:VAL:HG13	2.14	0.47
1:A:128:LEU:N	1:A:129:PRO:CD	2.77	0.47
1:B:85:VAL:HG11	1:B:98:ALA:HA	1.95	0.47
1:B:90:GLN:HG2	1:B:143:TYR:CZ	2.48	0.47
1:B:353:ASN:ND2	1:B:354:LEU:N	2.54	0.47
1:A:111:ARG:HG2	1:A:111:ARG:HH11	1.79	0.47
1:A:395:TYR:O	1:A:440:LEU:HA	2.14	0.47
1:A:407:LYS:C	1:A:409:ALA:H	2.22	0.47
1:A:538:THR:HG23	4:A:753:NAP:O5D	2.15	0.47
1:B:81:ARG:HG3	1:B:81:ARG:NH1	2.30	0.47
1:B:405:LEU:HA	1:B:408:MET:HE3	1.95	0.47
1:A:408:MET:HG3	1:A:419:TYR:HB2	1.97	0.47
1:B:484:LYS:C	1:B:486:GLY:H	2.22	0.47
1:B:570:ARG:HD3	1:B:575:ASP:OD2	2.15	0.47
1:B:96:GLU:OE2	1:B:96:GLU:HA	2.15	0.46
1:A:111:ARG:HG2	1:A:111:ARG:NH1	2.31	0.46
1:B:317:TYR:CD1	1:B:317:TYR:C	2.93	0.46
1:B:463:SER:HB3	1:B:473:HIS:HB2	1.97	0.46
1:A:339:LYS:HB3	1:A:339:LYS:HZ2	1.81	0.46
1:B:157:ASP:O	1:B:161:GLU:OE1	2.34	0.46
1:B:246:ARG:HD2	1:B:446:HIS:CE1	2.51	0.46
1:A:128:LEU:HD23	1:A:169:VAL:HG13	1.96	0.46
1:B:72:PHE:O	1:B:76:MET:HG3	2.16	0.45
1:B:265:GLU:HA	1:B:272:TYR:CD1	2.51	0.45
1:A:265:GLU:HA	1:A:272:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:LEU:C	1:B:441:ARG:HG3	2.40	0.45
1:B:231:CYS:SG	1:B:237:GLU:HA	2.56	0.45
1:B:91:THR:HB	3:B:751:FMN:O1P	2.16	0.45
1:B:155:PHE:CZ	1:B:159:LEU:HD11	2.51	0.45
1:A:644:ASN:HA	1:A:647:TYR:CD1	2.52	0.45
1:B:436:ASP:OD2	1:B:436:ASP:N	2.50	0.45
1:B:104:ASP:O	1:B:105:ALA:C	2.59	0.45
1:B:520:GLN:HE21	1:B:520:GLN:HA	1.81	0.45
1:B:665:ILE:HG22	1:B:669:MET:HE3	1.98	0.45
1:B:430:ILE:HG23	1:B:431:LEU:N	2.31	0.44
1:B:290:THR:HG23	1:B:309:ASP:HB2	1.99	0.44
1:A:175:GLY:C	1:A:185:ASN:HD21	2.26	0.44
1:B:290:THR:CG2	1:B:309:ASP:HB2	2.47	0.44
1:B:220:ILE:HG21	1:B:411:SER:HB3	1.99	0.44
1:B:543:PHE:HA	1:B:546:PHE:HB2	2.00	0.44
1:A:232:GLU:OE1	1:A:232:GLU:O	2.35	0.44
1:A:142:THR:CG2	1:A:146:GLY:HA2	2.48	0.44
1:A:517:ARG:HG3	1:A:517:ARG:HH11	1.83	0.44
1:A:635:ALA:HB2	1:A:678:VAL:HB	2.00	0.44
1:B:99:ASN:HD22	1:B:114:SER:HB2	1.82	0.44
1:B:246:ARG:HG3	1:B:246:ARG:HH11	1.83	0.43
1:B:355:ASP:C	1:B:357:GLU:H	2.26	0.43
1:B:571:ARG:HG2	1:B:571:ARG:HH11	1.83	0.43
1:A:178:ASN:HB3	1:A:181:TYR:HD2	1.82	0.43
1:B:238:ALA:O	1:B:239:THR:CB	2.66	0.43
1:B:121:ASP:C	1:B:123:ALA:H	2.25	0.43
1:A:389:LEU:HD13	1:A:408:MET:HE3	2.00	0.43
1:A:532:ILE:HD13	1:A:619:LEU:HD22	2.01	0.43
1:A:648:ASP:O	1:A:652:GLU:HG3	2.19	0.43
1:B:411:SER:O	1:B:412:SER:HB2	2.19	0.43
1:B:533:MET:HB3	1:B:543:PHE:CE1	2.53	0.43
1:A:224:GLU:OE2	1:A:411:SER:HB2	2.18	0.43
1:A:640:ARG:HE	1:A:640:ARG:HB3	1.43	0.43
1:A:216:GLU:OE2	1:A:386:THR:N	2.50	0.43
1:B:162:THR:OG1	1:B:164:VAL:HG13	2.19	0.43
1:B:405:LEU:HD23	1:B:408:MET:HE1	2.01	0.43
1:B:537:GLY:HA2	6:B:35:HOH:O	2.18	0.43
1:A:602:GLN:NE2	1:A:606:VAL:HG21	2.34	0.42
1:A:305:HIS:HE1	1:A:307:GLU:OE1	2.02	0.42
1:B:660:GLN:HE21	1:B:660:GLN:HB2	1.66	0.42
1:A:525:PHE:CD1	1:A:525:PHE:C	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:TYR:HE1	1:B:611:LEU:O	2.02	0.42
1:A:217:GLU:OE1	1:A:220:ILE:HD11	2.20	0.42
1:B:527:ALA:CB	1:B:553:LEU:HD13	2.49	0.42
1:A:467:VAL:HG12	1:A:468:HIS:CE1	2.55	0.42
1:B:634:ASP:O	1:B:638:MET:HE3	2.19	0.42
1:A:104:ASP:HB2	1:A:227:TRP:HZ2	1.85	0.42
1:A:461:ILE:HG22	1:A:463:SER:H	1.85	0.42
1:A:100:ARG:HD2	1:A:387:ASN:ND2	2.34	0.42
1:A:108:TYR:HD1	1:A:231:CYS:SG	2.43	0.42
1:B:317:TYR:O	1:B:465:SER:HB3	2.20	0.42
1:B:347:VAL:O	1:B:369:SER:HA	2.20	0.42
1:A:103:LYS:HE3	6:A:21:HOH:O	2.20	0.41
1:A:239:THR:C	1:A:241:GLU:H	2.28	0.41
1:B:317:TYR:O	1:B:465:SER:CB	2.68	0.41
1:A:144:GLY:HA2	6:A:7:HOH:O	2.21	0.41
1:B:216:GLU:OE1	1:B:385:ARG:HD3	2.20	0.41
1:B:305:HIS:CD2	1:B:578:TYR:OH	2.62	0.41
1:A:100:ARG:NH1	1:A:387:ASN:HD22	2.17	0.41
1:A:272:TYR:HE1	1:A:284:PRO:HG2	1.85	0.41
1:A:364:PHE:O	1:A:365:PRO:C	2.63	0.41
1:B:159:LEU:HB3	1:B:194:ARG:HG2	2.01	0.41
1:B:104:ASP:HB2	1:B:227:TRP:CZ2	2.55	0.41
1:B:248:TYR:CD2	1:B:353:ASN:HA	2.56	0.41
1:A:101:LEU:O	1:A:104:ASP:HB2	2.20	0.41
1:B:301:ARG:HD2	1:B:570:ARG:HH21	1.86	0.41
1:B:304:MET:CE	1:B:498:ARG:HA	2.45	0.41
1:B:323:VAL:HG12	1:B:459:TYR:O	2.21	0.41
1:B:629:ILE:HG21	1:B:646:PHE:CE1	2.55	0.41
1:B:85:VAL:HG22	1:B:137:VAL:HB	2.02	0.41
1:B:539:GLY:O	1:B:542:PRO:HD2	2.20	0.41
1:A:269:LEU:O	1:A:270:LYS:HB2	2.20	0.41
1:A:543:PHE:HA	1:A:546:PHE:HB2	2.03	0.41
1:A:555:GLN:C	1:A:557:GLY:H	2.28	0.41
1:A:572:SER:HB3	1:A:598:PHE:CZ	2.56	0.41
1:B:425:GLU:CG	1:B:484:LYS:NZ	2.83	0.41
1:B:501:GLU:HA	1:B:502:PRO:HD3	1.91	0.41
1:A:407:LYS:NZ	1:A:407:LYS:CB	2.83	0.41
1:A:407:LYS:C	1:A:409:ALA:N	2.75	0.41
1:B:90:GLN:CB	1:B:143:TYR:CZ	3.03	0.41
1:B:99:ASN:HD22	1:B:114:SER:CB	2.34	0.41
1:B:260:LYS:HA	1:B:269:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:THR:O	1:B:306:LEU:HA	2.21	0.41
1:B:353:ASN:ND2	1:B:353:ASN:C	2.78	0.41
1:B:427:ARG:HG2	1:B:427:ARG:HH21	1.86	0.41
1:B:551:ALA:HB2	1:B:590:ALA:HB1	2.03	0.41
1:A:294:LYS:HE3	1:A:296:ASN:O	2.21	0.41
1:B:404:LEU:HD23	1:B:404:LEU:C	2.46	0.41
1:B:520:GLN:HA	1:B:520:GLN:NE2	2.36	0.41
1:B:533:MET:HB3	1:B:543:PHE:CD1	2.56	0.41
1:A:517:ARG:HG3	1:A:517:ARG:NH1	2.36	0.40
1:A:644:ASN:O	1:A:647:TYR:HB2	2.21	0.40
1:A:104:ASP:CB	1:A:227:TRP:CZ2	3.04	0.40
1:B:99:ASN:HD22	1:B:99:ASN:HA	1.72	0.40
1:B:312:ASP:OD2	1:B:312:ASP:N	2.54	0.40
1:A:90:GLN:HB3	1:A:143:TYR:CZ	2.57	0.40
1:B:84:ILE:O	1:B:84:ILE:HG23	2.20	0.40
1:B:111:ARG:HH11	1:B:111:ARG:HG3	1.86	0.40
1:B:121:ASP:C	1:B:123:ALA:N	2.79	0.40
1:B:608:VAL:HG23	1:B:609:GLN:N	2.37	0.40
1:B:398:GLU:HA	1:B:399:PRO:HD3	1.91	0.40
1:B:459:TYR:HB3	1:B:474:ILE:HG23	2.04	0.40
1:B:527:ALA:HB1	1:B:553:LEU:HD13	2.04	0.40
1:B:617:GLU:HB2	6:B:24:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	600/618 (97%)	566 (94%)	32 (5%)	2 (0%)	36	50
1	B	597/618 (97%)	533 (89%)	55 (9%)	9 (2%)	8	12
All	All	1197/1236 (97%)	1099 (92%)	87 (7%)	11 (1%)	14	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLY
1	B	239	THR
1	B	356	GLU
1	A	408	MET
1	B	144	GLY
1	B	527	ALA
1	B	394	GLN
1	B	162	THR
1	B	485	ALA
1	B	246	ARG
1	B	616	ARG

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	510/525 (97%)	491 (96%)	19 (4%)	30	51
1	B	514/525 (98%)	492 (96%)	22 (4%)	26	44
All	All	1024/1050 (98%)	983 (96%)	41 (4%)	28	47

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	179	LYS
1	A	224	GLU
1	A	230	VAL
1	A	232	GLU
1	A	255	ASP
1	A	325	VAL
1	A	327	PRO
1	A	339	LYS
1	A	404	LEU
1	A	407	LYS
1	A	408	MET

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Mol	Chain	Res	Type
1	A	418	LEU
1	A	429	HIS
1	A	441	ARG
1	A	591	LEU
1	A	602	GLN
1	A	609	GLN
1	A	640	ARG
1	B	78	LYS
1	B	111	ARG
1	B	203	ILE
1	B	228	PRO
1	B	270	LYS
1	B	273	GLU
1	B	297	GLN
1	B	337	LEU
1	B	403	GLU
1	B	407	LYS
1	B	425	GLU
1	B	436	ASP
1	B	481	TYR
1	B	511	LEU
1	B	531	VAL
1	B	540	VAL
1	B	556	GLN
1	B	570	ARG
1	B	591	LEU
1	B	609	GLN
1	B	640	ARG
1	B	667	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	185	ASN
1	A	201	GLN
1	A	233	HIS
1	A	253	HIS
1	A	283	ASN
1	A	297	GLN
1	A	305	HIS
1	A	353	ASN

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Mol	Chain	Res	Type
1	A	362	HIS
1	A	382	ASN
1	A	387	ASN
1	A	394	GLN
1	A	429	HIS
1	A	435	GLN
1	A	446	HIS
1	A	489	ASN
1	A	555	GLN
1	A	556	GLN
1	A	584	GLN
1	A	586	HIS
1	A	593	GLN
1	A	595	ASN
1	A	602	GLN
1	A	609	GLN
1	A	637	ASN
1	A	660	GLN
1	B	90	GLN
1	B	99	ASN
1	B	133	ASN
1	B	153	GLN
1	B	183	HIS
1	B	185	ASN
1	B	233	HIS
1	B	247	GLN
1	B	275	GLN
1	B	283	ASN
1	B	297	GLN
1	B	305	HIS
1	B	322	HIS
1	B	329	ASN
1	B	353	ASN
1	B	402	GLN
1	B	435	GLN
1	B	455	GLN
1	B	468	HIS
1	B	489	ASN
1	B	520	GLN
1	B	555	GLN
1	B	584	GLN
1	B	586	HIS

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Mol	Chain	Res	Type
1	B	593	GLN
1	B	604	HIS
1	B	609	GLN
1	B	660	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	FMN	B	751	-	33,33,33	2.32	11 (33%)	48,50,50	1.51	10 (20%)
3	FMN	A	751	-	33,33,33	2.47	12 (36%)	48,50,50	1.47	8 (16%)
4	NAP	B	753	-	32,33,52	2.59	10 (31%)	50,52,80	2.02	12 (24%)
4	NAP	A	753	-	32,33,52	2.80	11 (34%)	50,52,80	2.02	12 (24%)
2	FAD	B	752	-	58,58,58	2.92	22 (37%)	85,89,89	1.52	14 (16%)
2	FAD	A	752	-	58,58,58	2.76	21 (36%)	85,89,89	1.55	13 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	B	751	-	-	0/18/18/18	0/3/3/3
3	FMN	A	751	-	-	0/18/18/18	0/3/3/3
4	NAP	B	753	-	-	3/21/37/67	0/3/3/5
4	NAP	A	753	-	-	4/21/37/67	0/3/3/5
2	FAD	B	752	-	-	2/34/50/50	0/6/6/6
2	FAD	A	752	-	-	4/34/50/50	0/6/6/6

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	752	FAD	PA-O3P	-9.37	1.49	1.59
4	A	753	NAP	C4A-N3A	8.87	1.51	1.34
4	B	753	NAP	C4A-N3A	8.33	1.50	1.34
2	A	752	FAD	PA-O3P	-8.23	1.50	1.59
4	A	753	NAP	PA-O3	-8.06	1.50	1.59
4	B	753	NAP	PA-O3	-7.34	1.51	1.59
2	B	752	FAD	C5'-C4'	-6.65	1.42	1.51
2	B	752	FAD	C4A-N3A	6.50	1.46	1.34
2	B	752	FAD	C1'-C2'	6.34	1.61	1.52
2	A	752	FAD	C4A-N3A	6.05	1.45	1.34
2	A	752	FAD	C1'-C2'	5.95	1.60	1.52
2	A	752	FAD	C5'-C4'	-5.94	1.43	1.51
2	A	752	FAD	C9A-N10	5.78	1.51	1.41
2	B	752	FAD	C9A-C5X	5.58	1.50	1.41
3	A	751	FMN	C10-N10	5.55	1.49	1.37
3	B	751	FMN	C10-N10	5.52	1.49	1.37
4	A	753	NAP	C5A-C4A	5.29	1.48	1.39
3	A	751	FMN	C4A-N5	5.07	1.41	1.30
4	B	753	NAP	C5A-C4A	4.69	1.47	1.39
2	A	752	FAD	C9A-C5X	4.66	1.48	1.41
2	B	752	FAD	C9A-N10	4.65	1.49	1.41
3	B	751	FMN	C4A-N5	4.64	1.40	1.30
3	B	751	FMN	C9A-N10	4.58	1.49	1.41
2	B	752	FAD	C4X-N5	4.53	1.40	1.30
3	A	751	FMN	C9A-N10	4.45	1.48	1.41
2	A	752	FAD	C4X-N5	4.42	1.40	1.30
3	A	751	FMN	C9-C9A	4.42	1.46	1.39
2	A	752	FAD	C6-C5X	4.35	1.46	1.40
2	B	752	FAD	C6-C5X	4.25	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	752	FAD	C8A-N7A	4.21	1.39	1.31
2	A	752	FAD	C2'-C3'	4.20	1.60	1.53
3	B	751	FMN	C9-C9A	4.18	1.46	1.39
2	A	752	FAD	C8A-N7A	4.14	1.39	1.31
2	B	752	FAD	C8-C7	4.06	1.50	1.40
3	A	751	FMN	C1'-C2'	4.05	1.58	1.52
2	B	752	FAD	C5A-C4A	4.00	1.46	1.39
3	A	751	FMN	C9A-C5A	3.98	1.47	1.41
3	A	751	FMN	C8-C7	3.94	1.50	1.40
2	A	752	FAD	C5A-C4A	3.80	1.45	1.39
4	A	753	NAP	P2B-O1X	3.78	1.62	1.50
2	B	752	FAD	C2'-C3'	3.76	1.60	1.53
3	B	751	FMN	C9A-C5A	3.71	1.47	1.41
4	B	753	NAP	P2B-O1X	3.66	1.61	1.50
2	A	752	FAD	C10-N1	3.64	1.40	1.33
2	B	752	FAD	C10-N1	3.58	1.40	1.33
3	A	751	FMN	C6-C5A	3.47	1.45	1.40
3	B	751	FMN	C8-C7	3.44	1.49	1.40
3	B	751	FMN	C1'-C2'	3.35	1.57	1.52
4	A	753	NAP	C8A-N7A	3.24	1.37	1.31
2	B	752	FAD	P-O3P	-3.22	1.56	1.59
2	B	752	FAD	C6-C7	3.19	1.44	1.39
2	A	752	FAD	C8-C7	3.10	1.48	1.40
2	A	752	FAD	P-O3P	-3.07	1.56	1.59
2	B	752	FAD	O2'-C2'	3.05	1.49	1.43
3	B	751	FMN	C6-C5A	2.98	1.44	1.40
2	A	752	FAD	C9-C9A	2.98	1.44	1.39
4	B	753	NAP	C8A-N7A	2.98	1.37	1.31
4	B	753	NAP	PA-O5B	-2.96	1.47	1.59
4	A	753	NAP	C2A-N1A	2.94	1.39	1.33
2	B	752	FAD	PA-O5B	-2.91	1.48	1.59
2	B	752	FAD	P-O5'	-2.88	1.48	1.59
2	B	752	FAD	C9-C9A	2.87	1.44	1.39
2	B	752	FAD	C4-N3	2.86	1.44	1.38
2	A	752	FAD	P-O5'	-2.77	1.48	1.59
2	A	752	FAD	C4-N3	2.73	1.44	1.38
3	B	751	FMN	C4'-C3'	2.71	1.58	1.53
4	A	753	NAP	C8A-N9A	2.70	1.42	1.37
2	A	752	FAD	C6-C7	2.67	1.43	1.39
4	A	753	NAP	PA-O5B	-2.65	1.49	1.59
3	A	751	FMN	C4'-C3'	2.58	1.57	1.53
4	A	753	NAP	P2B-O2B	2.57	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	752	FAD	O2'-C2'	2.52	1.48	1.43
3	B	751	FMN	C10-N1	2.50	1.38	1.33
4	B	753	NAP	C2A-N1A	2.49	1.38	1.33
3	A	751	FMN	O4'-C4'	2.45	1.48	1.43
4	B	753	NAP	C1B-N9A	-2.43	1.39	1.46
2	B	752	FAD	C2A-N3A	2.37	1.38	1.33
4	A	753	NAP	C1B-N9A	-2.36	1.39	1.46
2	A	752	FAD	PA-O5B	-2.27	1.50	1.59
4	A	753	NAP	C5A-C6A	2.26	1.47	1.41
4	B	753	NAP	C5A-C6A	2.23	1.47	1.41
3	A	751	FMN	C10-N1	2.17	1.37	1.33
3	B	751	FMN	C7M-C7	2.12	1.55	1.51
2	A	752	FAD	C2A-N3A	2.12	1.37	1.33
3	A	751	FMN	C8M-C8	2.06	1.54	1.51
4	B	753	NAP	C8A-N9A	2.04	1.41	1.37
2	B	752	FAD	C5A-C6A	2.01	1.46	1.41

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	753	NAP	N9A-C8A-N7A	6.05	122.53	113.94
4	A	753	NAP	N9A-C8A-N7A	6.03	122.49	113.94
4	B	753	NAP	C4A-N9A-C8A	-5.84	99.60	105.74
4	A	753	NAP	C4A-N9A-C8A	-5.70	99.75	105.74
2	B	752	FAD	C2A-N1A-C6A	5.59	127.91	118.73
2	A	752	FAD	C2A-N1A-C6A	5.58	127.89	118.73
4	B	753	NAP	C5A-C4A-N3A	-5.09	119.70	126.72
4	A	753	NAP	C5A-C4A-N3A	-4.81	120.10	126.72
2	B	752	FAD	N3A-C2A-N1A	-4.33	122.03	128.58
2	A	752	FAD	N3A-C2A-N1A	-4.31	122.06	128.58
4	A	753	NAP	C5A-N7A-C8A	-4.18	96.88	103.45
4	B	753	NAP	C5A-N7A-C8A	-4.09	97.02	103.45
3	B	751	FMN	C9A-C5A-N5	4.06	126.77	122.45
3	A	751	FMN	C9A-C5A-N5	3.76	126.44	122.45
4	A	753	NAP	C1B-N9A-C8A	3.58	135.03	127.09
4	B	753	NAP	C1B-N9A-C8A	3.40	134.64	127.09
2	A	752	FAD	C1B-N9A-C8A	3.31	134.44	127.09
3	A	751	FMN	O4-C4-N3	-3.30	113.91	120.11
4	A	753	NAP	N3A-C2A-N1A	-3.14	123.83	128.58
2	B	752	FAD	O2P-P-O3P	3.09	115.64	107.27
2	A	752	FAD	C2'-C1'-N10	-3.07	95.71	110.20
3	B	751	FMN	O4-C4-N3	-3.00	114.47	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	753	NAP	N3A-C2A-N1A	-3.00	124.04	128.58
2	B	752	FAD	C2'-C1'-N10	-3.00	96.02	110.20
2	B	752	FAD	O2-C2-N3	2.99	124.32	118.58
2	A	752	FAD	O2-C2-N3	2.98	124.31	118.58
4	B	753	NAP	N3A-C4A-N9A	2.97	132.22	127.17
2	A	752	FAD	C5X-C9A-N10	-2.91	115.33	117.97
4	A	753	NAP	N3A-C4A-N9A	2.86	132.03	127.17
2	A	752	FAD	C9-C9A-N10	2.83	125.67	121.85
2	B	752	FAD	C1B-N9A-C8A	2.79	133.29	127.09
2	B	752	FAD	C8M-C8-C9	-2.77	114.69	119.57
2	A	752	FAD	C4A-N9A-C1B	-2.71	120.30	126.63
4	A	753	NAP	O2N-PN-O3	2.67	113.59	104.64
4	B	753	NAP	O4B-C1B-C2B	-2.67	101.99	106.59
4	B	753	NAP	O2N-PN-O3	2.60	113.34	104.64
4	A	753	NAP	C2A-N1A-C6A	2.55	122.92	118.73
2	B	752	FAD	C10-N1-C2	2.54	122.35	116.85
3	B	751	FMN	C9-C9A-N10	2.52	125.24	121.85
2	A	752	FAD	O2P-P-O3P	2.49	114.00	107.27
2	B	752	FAD	C5X-C9A-N10	-2.46	115.74	117.97
3	A	751	FMN	C5A-C9A-N10	-2.45	115.75	117.97
2	A	752	FAD	C10-N1-C2	2.45	122.15	116.85
4	B	753	NAP	O2A-PA-O3	2.44	113.88	107.27
4	B	753	NAP	C2A-N1A-C6A	2.44	122.73	118.73
2	B	752	FAD	C9A-C5X-N5	2.43	125.04	122.45
3	A	751	FMN	O4'-C4'-C3'	-2.38	103.67	109.25
4	A	753	NAP	O2A-PA-O3	2.37	113.69	107.27
2	B	752	FAD	O2A-PA-O3P	2.36	113.65	107.27
2	A	752	FAD	C9A-C5X-N5	2.34	124.94	122.45
3	B	751	FMN	C4'-C3'-C2'	-2.33	109.70	113.57
3	B	751	FMN	C5A-C9A-N10	-2.32	115.87	117.97
3	A	751	FMN	C8M-C8-C7	2.29	125.43	120.76
3	A	751	FMN	C8M-C8-C9	-2.24	115.62	119.57
2	B	752	FAD	C9-C9A-N10	2.22	124.84	121.85
2	A	752	FAD	C8M-C8-C9	-2.21	115.68	119.57
3	A	751	FMN	C9-C9A-N10	2.18	124.79	121.85
2	A	752	FAD	O3'-C3'-C2'	2.16	113.85	108.93
2	B	752	FAD	O2'-C2'-C3'	-2.15	104.22	109.25
3	B	751	FMN	C8M-C8-C9	-2.14	115.80	119.57
3	B	751	FMN	C6-C5A-N5	-2.14	114.89	118.44
3	B	751	FMN	C8M-C8-C7	2.12	125.09	120.76
4	A	753	NAP	C4A-C5A-N7A	2.12	113.00	110.58
4	A	753	NAP	O4B-C1B-C2B	-2.11	102.95	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	751	FMN	O2'-C2'-C3'	2.10	114.16	109.25
4	B	753	NAP	C5A-C4A-N9A	2.07	108.07	105.81
3	A	751	FMN	O2'-C2'-C3'	2.03	114.00	109.25
3	B	751	FMN	O3P-P-O5'	-2.02	101.40	106.67
2	B	752	FAD	C4A-N9A-C1B	-2.02	121.91	126.63

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	753	NAP	C2B-C1B-N9A-C8A
4	A	753	NAP	C2B-C1B-N9A-C8A
2	A	752	FAD	PA-O3P-P-O2P
2	B	752	FAD	PA-O3P-P-O2P
4	A	753	NAP	C2B-C1B-N9A-C4A
4	B	753	NAP	C2B-C1B-N9A-C4A
4	A	753	NAP	O4B-C1B-N9A-C8A
2	A	752	FAD	O2'-C2'-C3'-C4'
4	B	753	NAP	O4B-C1B-N9A-C8A
2	A	752	FAD	O2'-C2'-C3'-O3'
2	A	752	FAD	PA-O3P-P-O1P
2	B	752	FAD	PA-O3P-P-O1P
4	A	753	NAP	C2B-O2B-P2B-O3X

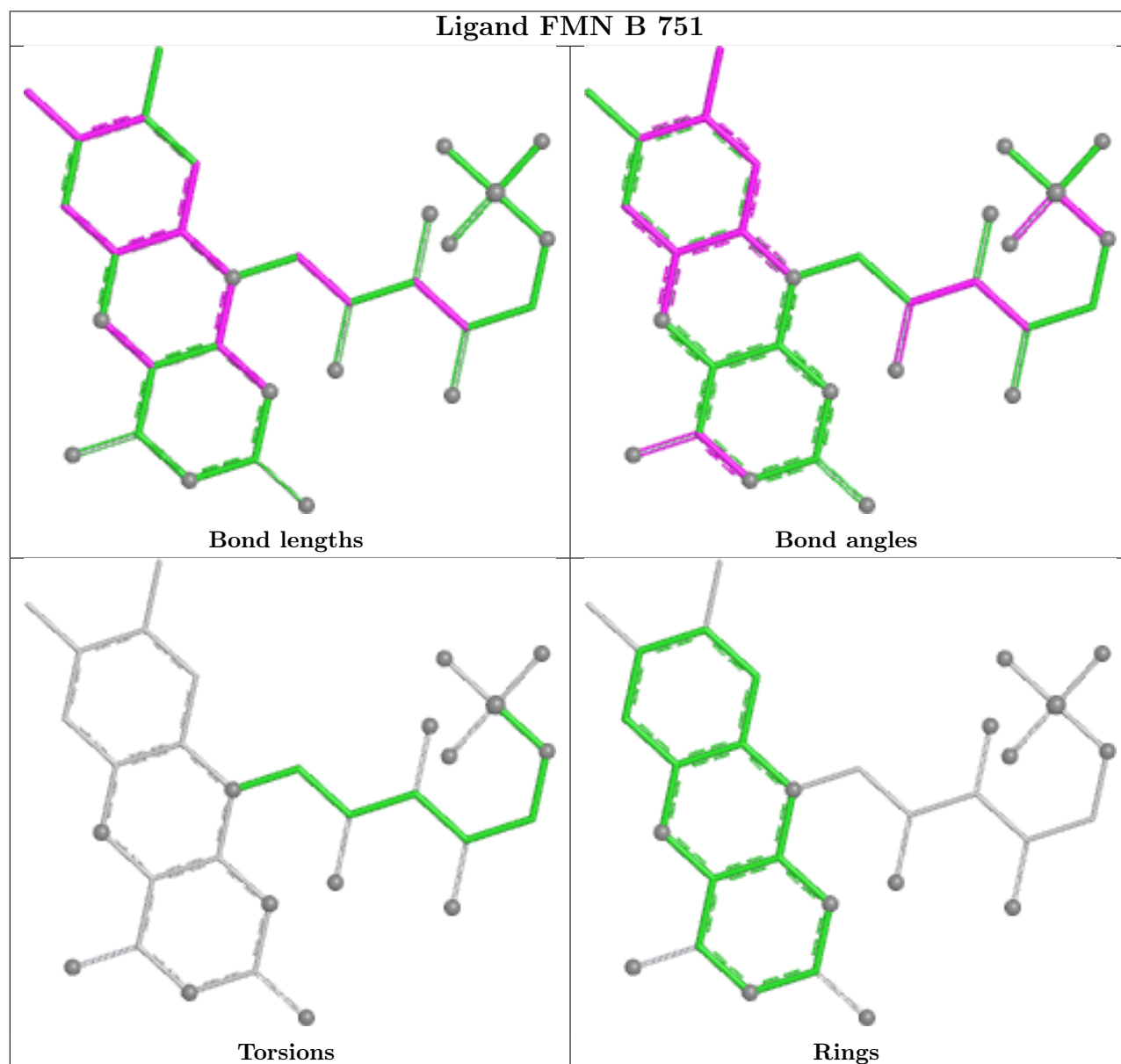
There are no ring outliers.

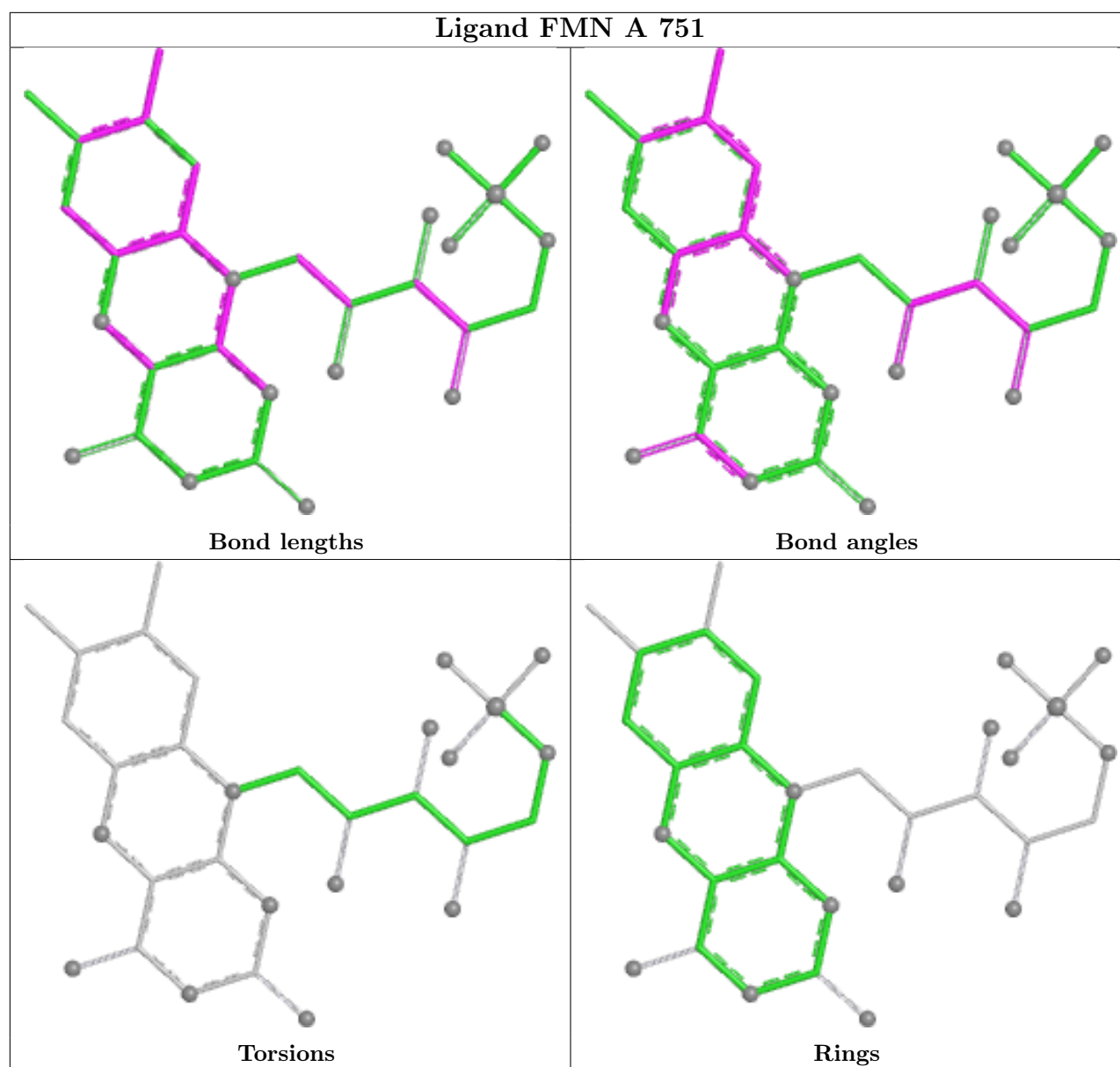
3 monomers are involved in 4 short contacts:

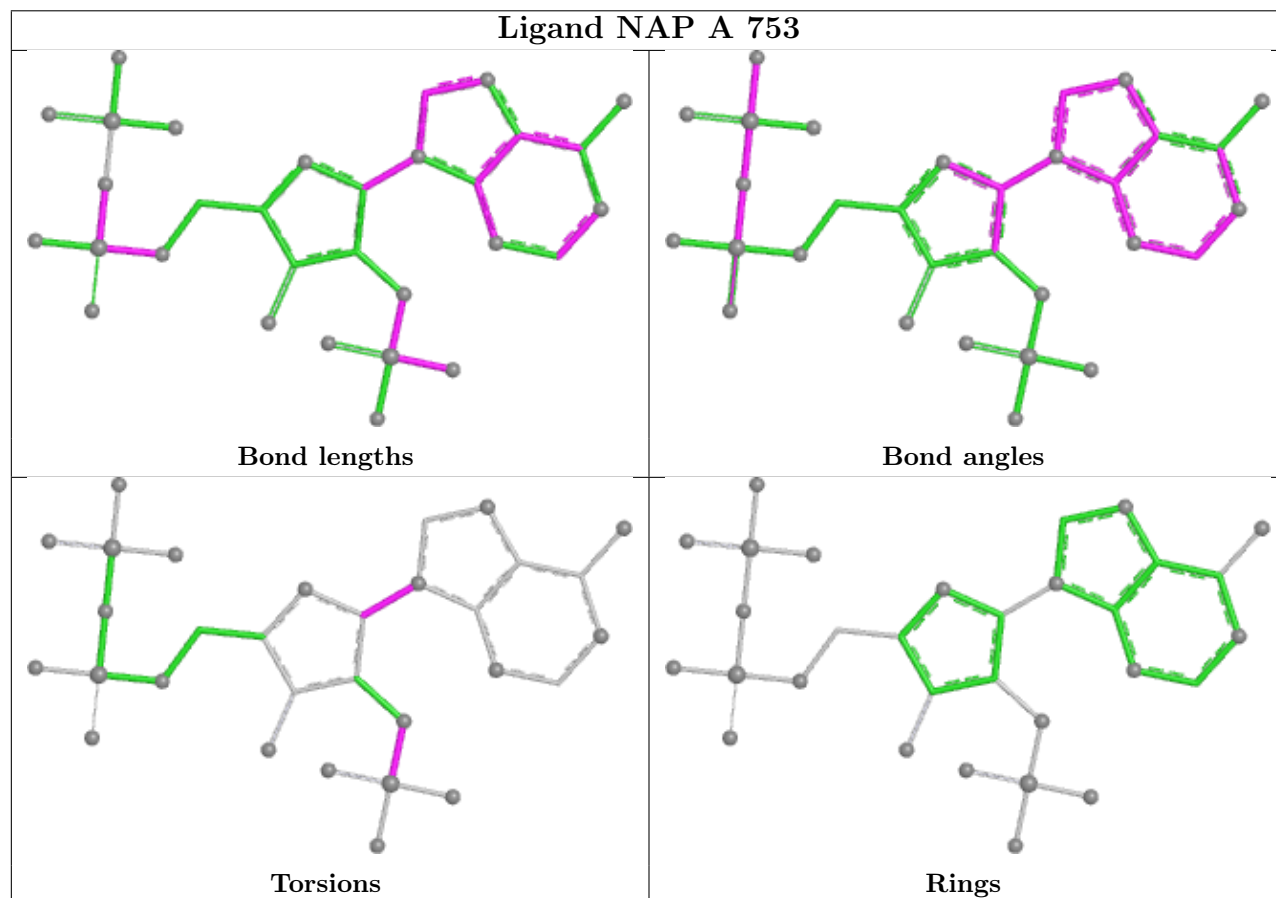
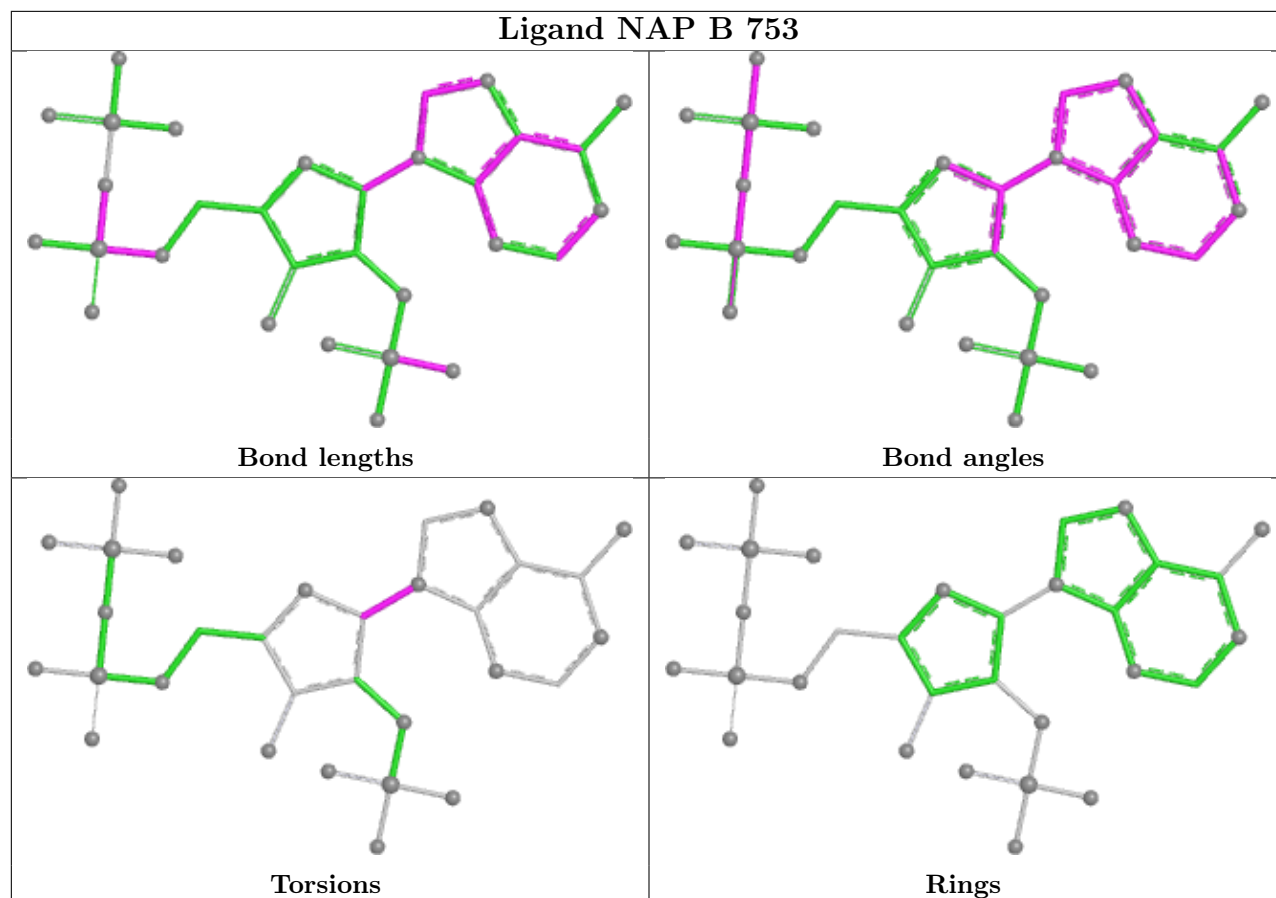
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	751	FMN	1	0
4	B	753	NAP	1	0
4	A	753	NAP	2	0

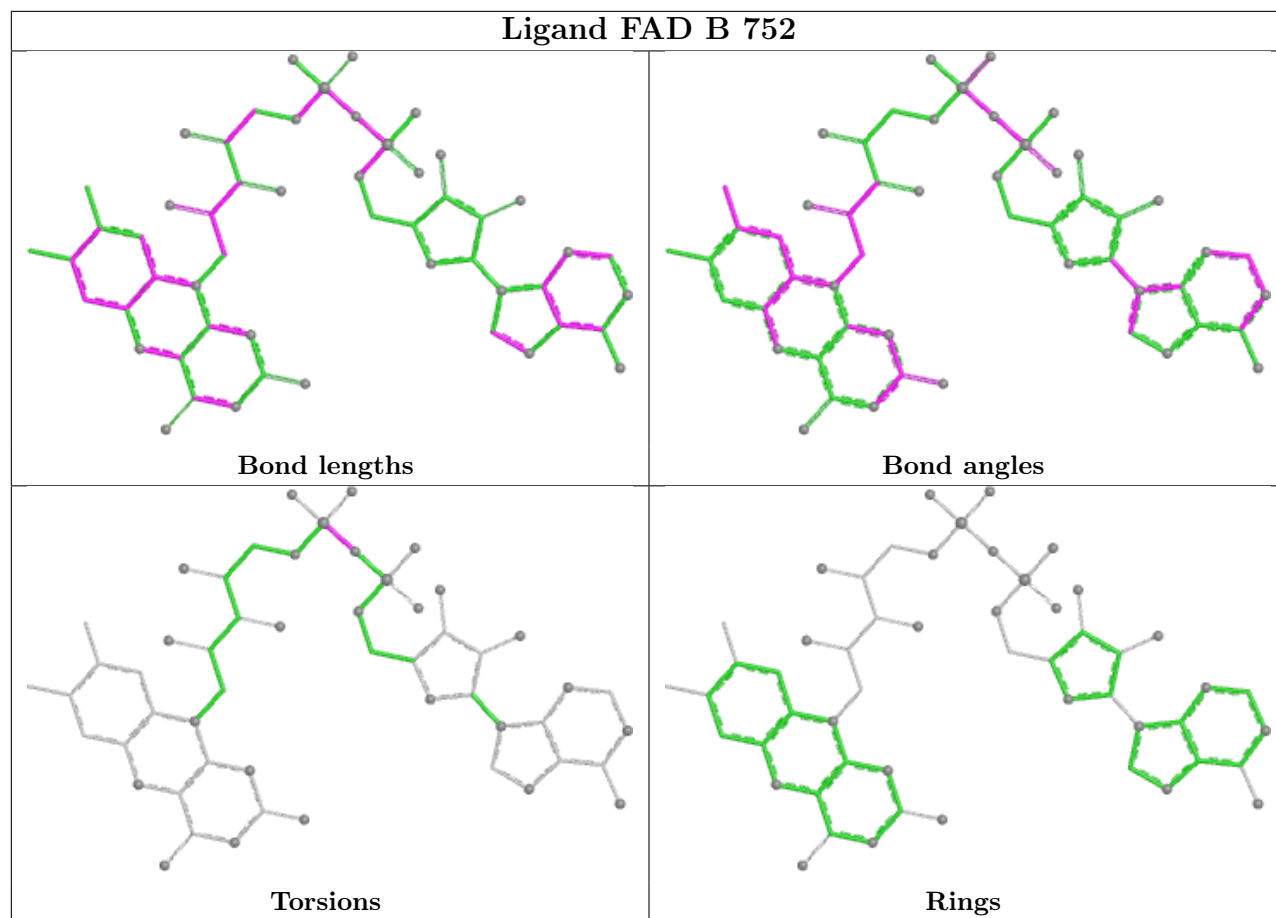
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

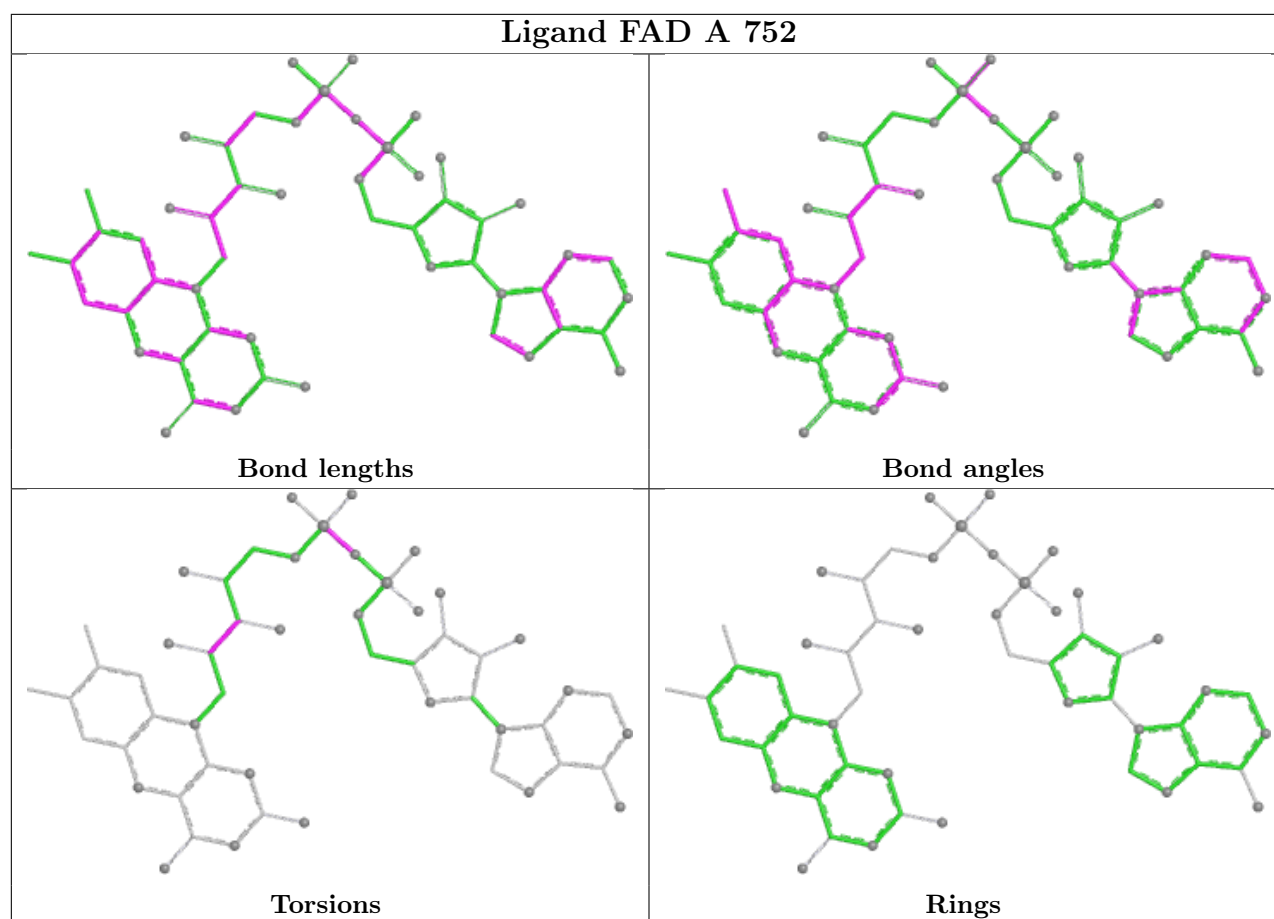
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	604/618 (97%)	-0.03	7 (1%) 76 73	35, 52, 78, 92	0
1	B	603/618 (97%)	0.33	16 (2%) 56 52	41, 65, 83, 90	0
All	All	1207/1236 (97%)	0.15	23 (1%) 66 62	35, 59, 82, 92	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	SER	3.2
1	A	243	SER	3.0
1	B	590	ALA	2.8
1	A	241	GLU	2.8
1	B	239	THR	2.7
1	B	254	THR	2.7
1	A	399	PRO	2.6
1	B	143	TYR	2.6
1	A	510	ALA	2.6
1	B	70	SER	2.5
1	B	245	ILE	2.4
1	B	481	TYR	2.4
1	B	92	GLY	2.3
1	B	358	SER	2.3
1	B	240	GLY	2.2
1	A	404	LEU	2.2
1	B	594	LEU	2.2
1	A	242	GLU	2.2
1	B	589	GLY	2.2
1	B	525	PHE	2.1
1	B	588	ASP	2.0
1	B	243	SER	2.0
1	B	564	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

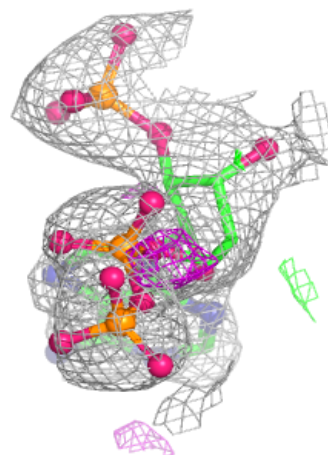
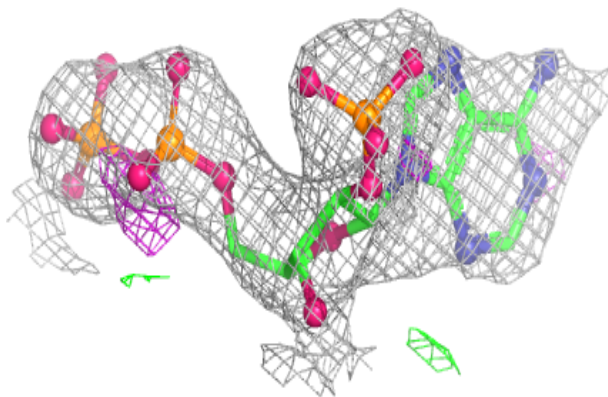
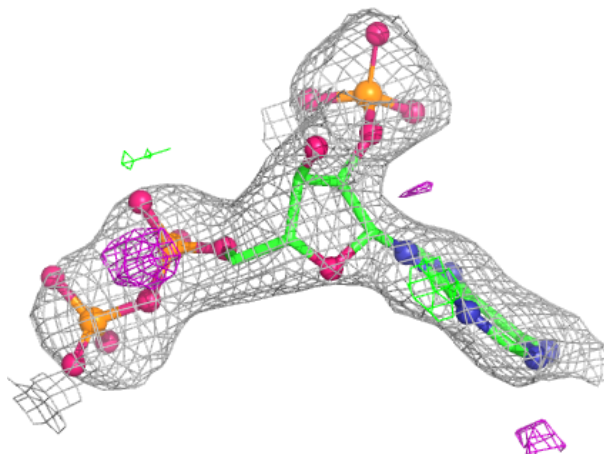
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	A	761	1/1	0.79	0.17	89,89,89,89	0
4	NAP	A	753	31/48	0.88	0.11	81,85,107,111	0
4	NAP	B	753	31/48	0.90	0.11	69,73,93,97	0
2	FAD	B	752	53/53	0.91	0.11	58,73,82,83	0
3	FMN	B	751	31/31	0.93	0.10	61,67,73,74	0
2	FAD	A	752	53/53	0.96	0.07	37,43,60,63	0
3	FMN	A	751	31/31	0.97	0.06	45,50,57,59	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.

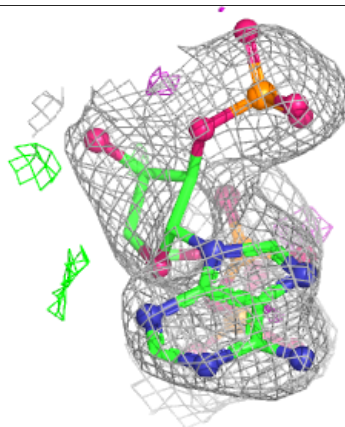
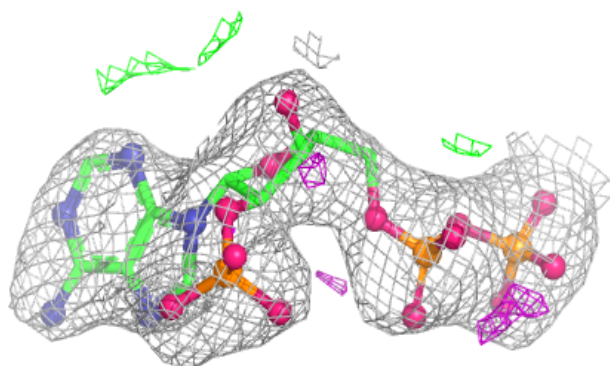
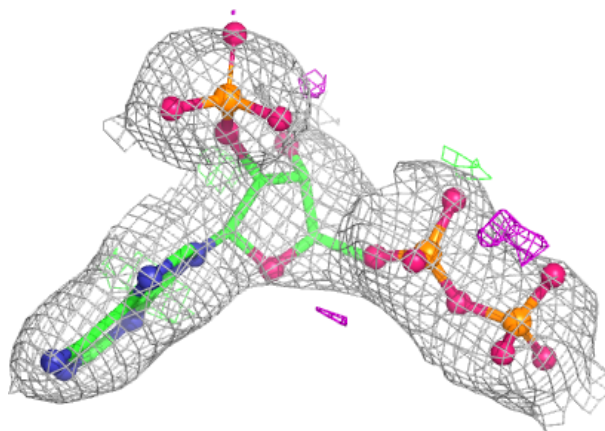
Electron density around NAP A 753:

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

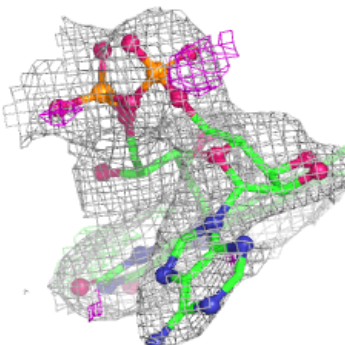
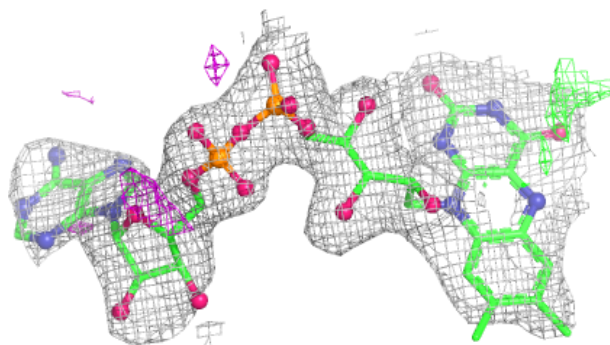
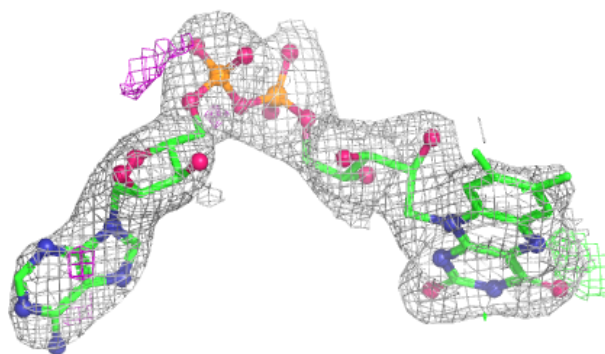


Electron density around NAP B 753:

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

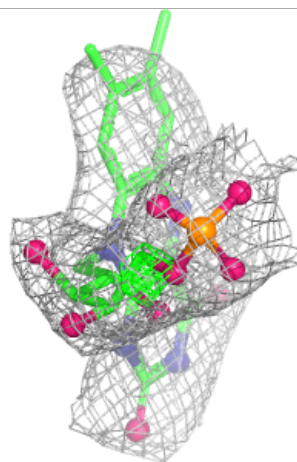
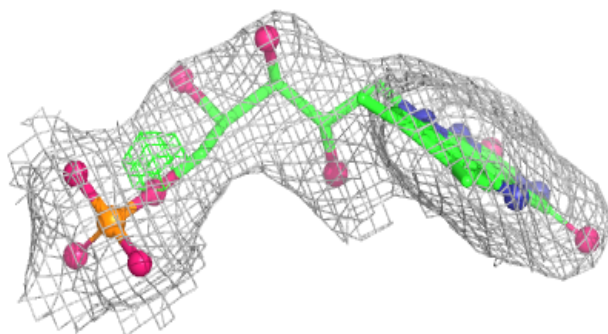
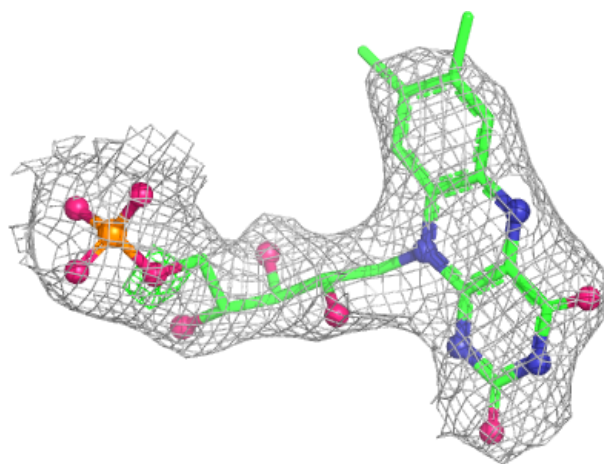
**Electron density around FAD B 752:**

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



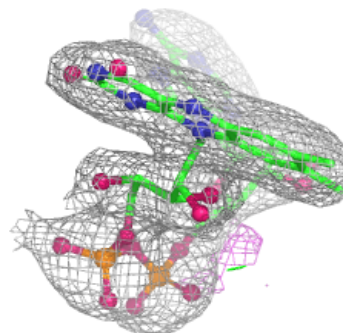
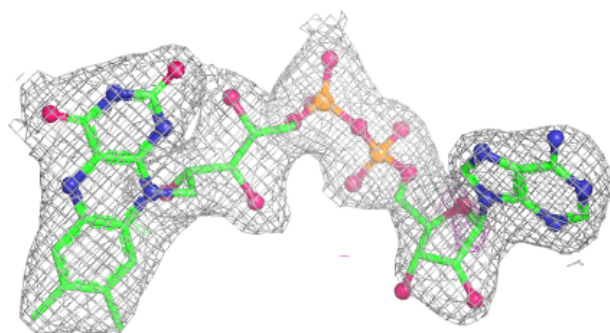
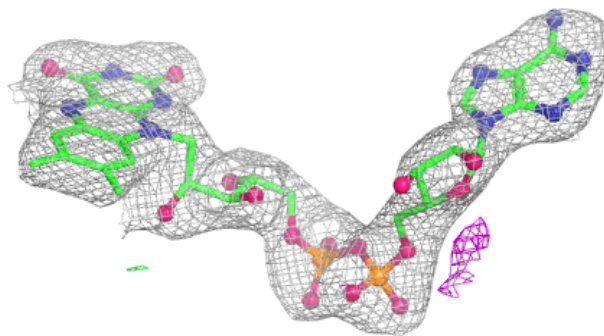
Electron density around FMN B 751:

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



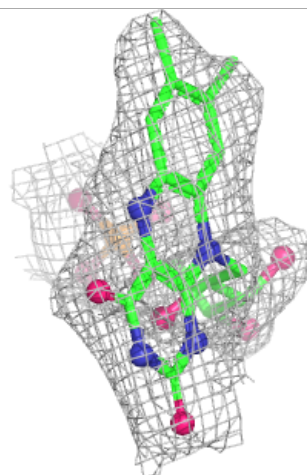
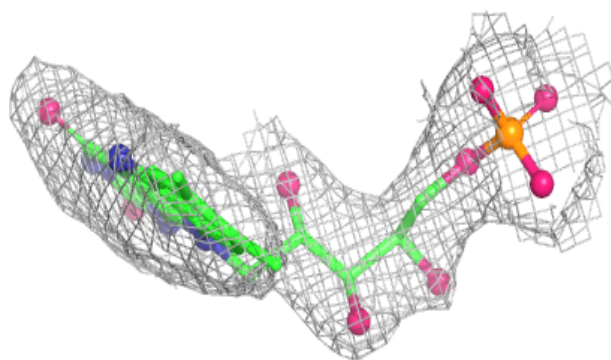
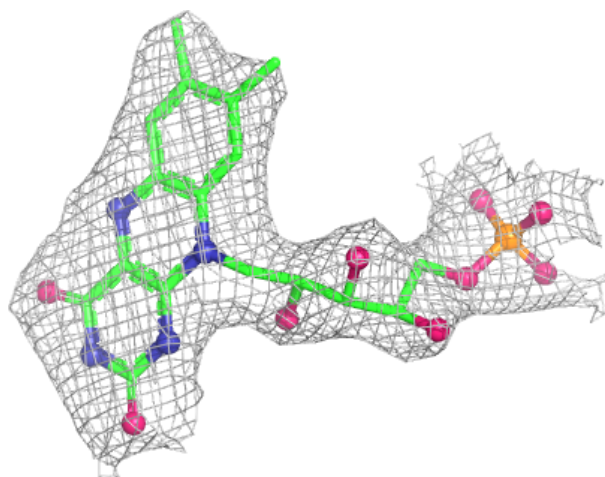
Electron density around FAD A 752:

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



Electron density around FMN A 751:

$2mF_o-DF_c$ (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.