



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:35 PM UTC

PDB ID : 3UP5 / pdb_00003up5
Title : Crystal Structure of OTEMO complex with FAD and NADP (form 4)
Authors : Shi, R.; Matte, A.; Cygler, M.; Lau, P.
Deposited on : 2011-11-17
Resolution : 2.45 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

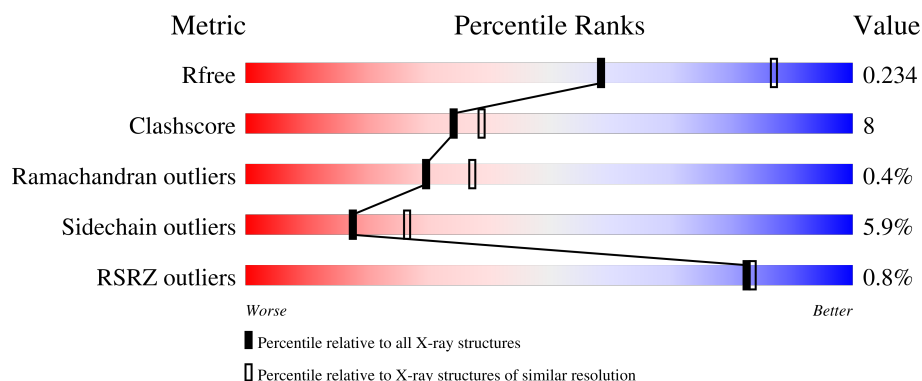
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	545	% 79% 16% ..
1	B	545	% 76% 19% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9004 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 OTEMO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	1	0
			4269	2712	736	807	14			
1	B	532	Total	C	N	O	S	0	2	0
			4235	2692	730	798	15			

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



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

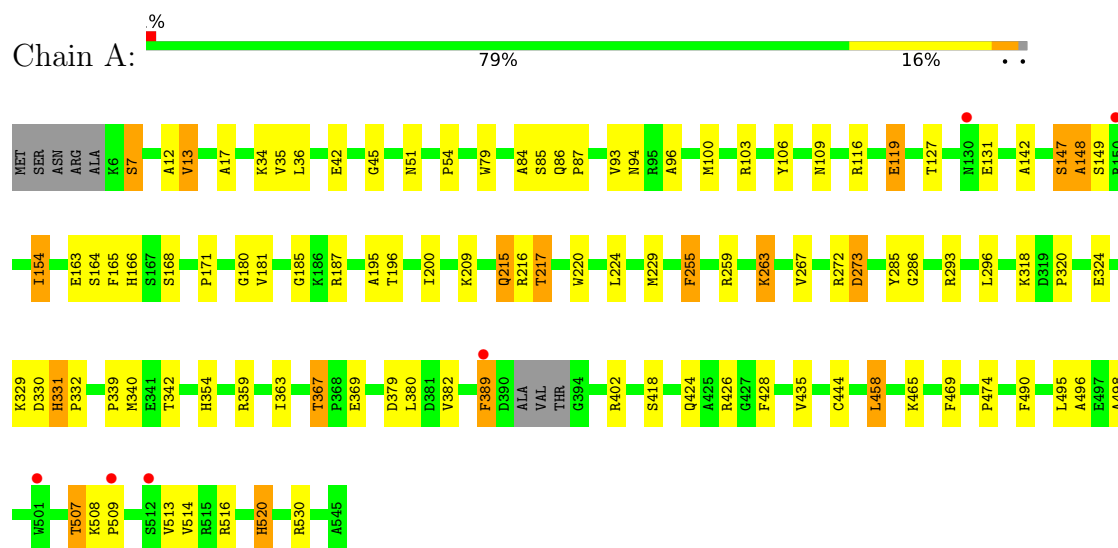
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	134	Total O 134 134	0	0
4	B	164	Total O 164 164	0	0

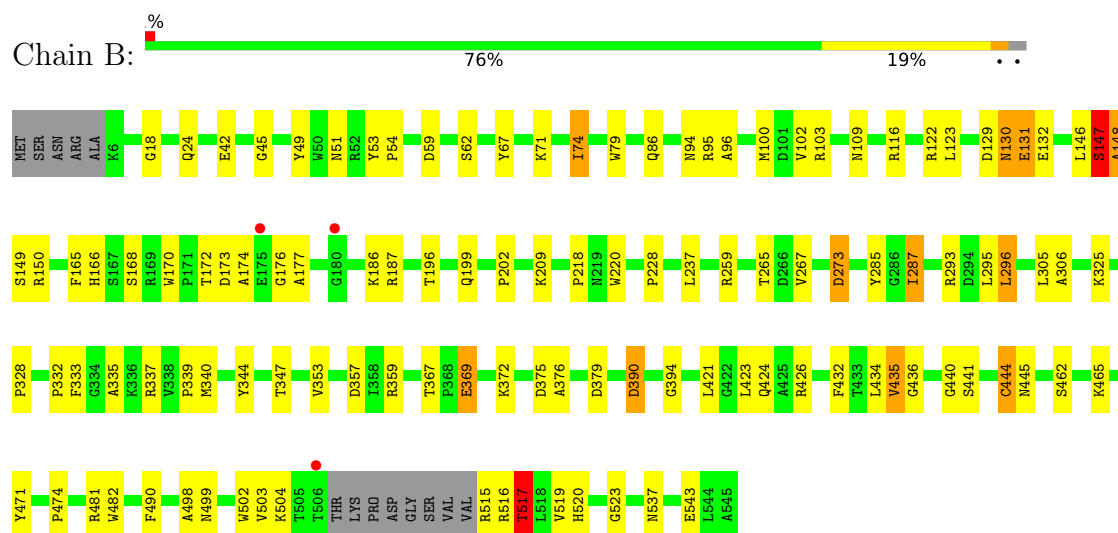
3 Residue-property plots [i](#)

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

• Molecule 1: OTEMO



• Molecule 1: OTEMO



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.84Å 94.39Å 93.14Å 90.00° 102.38° 90.00°	Depositor
Resolution (Å)	48.35 – 2.45 48.35 – 2.45	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.35-2.45) 96.2 (48.35-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 2.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.236 0.184 , 0.234	Depositor DCC
R_{free} test set	2019 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.904	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.4	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	0.94	EDS
Total number of atoms	9004	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% 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: 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	1.11	2/4382 (0.0%)	1.19	13/5953 (0.2%)
1	B	1.13	3/4350 (0.1%)	1.19	20/5909 (0.3%)
All	All	1.12	5/8732 (0.1%)	1.19	33/11862 (0.3%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	435	VAL	CA-CB	6.43	1.63	1.54
1	A	127	THR	CA-CB	5.89	1.61	1.53
1	B	147	SER	C-O	5.39	1.30	1.23
1	A	498	ALA	CA-CB	-5.30	1.45	1.53
1	B	228	PRO	C-O	-5.16	1.18	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	HIS	N-CA-C	11.40	118.48	108.22
1	A	142	ALA	N-CA-C	-8.37	100.54	110.41
1	B	498	ALA	N-CA-C	8.18	120.53	108.60
1	B	147	SER	N-CA-C	-8.02	97.09	109.52
1	A	255	PHE	CA-C-N	-7.55	111.72	121.91
1	A	255	PHE	C-N-CA	-7.55	111.72	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ASP	N-CA-C	7.54	119.14	111.07
1	A	428	PHE	CA-C-N	-7.30	112.80	120.03
1	A	428	PHE	C-N-CA	-7.30	112.80	120.03
1	A	84	ALA	N-CA-C	7.09	119.45	110.24
1	B	367	THR	CA-C-N	-6.43	113.18	119.87
1	B	367	THR	C-N-CA	-6.43	113.18	119.87
1	A	147	SER	N-CA-C	6.06	118.16	108.41
1	B	435	VAL	CB-CA-C	6.01	121.14	111.29
1	B	462	SER	N-CA-C	5.68	117.15	111.07
1	B	517	THR	N-CA-C	5.61	118.58	110.28
1	B	209	LYS	N-CA-C	-5.55	105.15	111.14
1	B	519	VAL	N-CA-C	5.54	116.72	108.46
1	B	186	LYS	N-CA-C	5.46	118.96	110.17
1	B	436	GLY	CA-C-N	5.42	126.26	120.13
1	B	436	GLY	C-N-CA	5.42	126.26	120.13
1	A	200	ILE	N-CA-C	5.39	116.12	110.62
1	B	523	GLY	N-CA-C	5.38	118.25	112.33
1	A	7	SER	CA-C-N	5.38	125.33	119.78
1	A	7	SER	C-N-CA	5.38	125.33	119.78
1	B	375	ASP	N-CA-C	5.26	119.83	113.41
1	B	237	LEU	N-CA-C	5.14	117.28	111.11
1	B	273	ASP	CA-C-N	5.14	127.58	120.29
1	B	273	ASP	C-N-CA	5.14	127.58	120.29
1	A	148	ALA	N-CA-C	5.09	121.65	110.80
1	B	359	ARG	N-CA-C	-5.03	105.88	111.36
1	B	376	ALA	N-CA-C	5.02	116.70	109.07
1	B	306	ALA	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	444	CYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4269	0	4113	66	0
1	B	4235	0	4085	62	0
2	A	53	0	31	0	0
2	B	53	0	31	2	0
3	A	48	0	25	1	0
3	B	48	0	25	2	0
4	A	134	0	0	7	0
4	B	164	0	0	8	0
All	All	9004	0	8310	130	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 8.

All (130) 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:94:ASN:HD22	1:A:103:ARG:HH21	1.07	0.98
2:B:551:FAD:O1P	4:B:685:HOH:O	1.84	0.96
1:A:367:THR:HG22	1:A:369:GLU:H	1.30	0.94
1:A:149:SER:HB3	1:A:168:SER:OG	1.71	0.90
1:B:537:ASN:HB2	4:B:612:HOH:O	1.71	0.89
1:B:424:GLN:HE21	1:B:474:PRO:HD3	1.40	0.86
1:A:181:VAL:N	4:A:646:HOH:O	2.14	0.79
1:A:224:LEU:CD1	1:A:340:MET:HE3	2.13	0.77
1:A:424:GLN:HE21	1:A:474:PRO:HD3	1.48	0.77
1:B:259:ARG:HH22	1:B:296:LEU:HD22	1.49	0.77
1:B:96:ALA:O	1:B:100:MET:HG3	1.88	0.74
1:B:94:ASN:HD22	1:B:103:ARG:HH21	1.34	0.74
1:B:18:GLY:CA	4:B:685:HOH:O	2.36	0.73
1:B:199:GLN:OE1	3:B:552:NAP:H4N	1.90	0.72
1:B:42:GLU:HG2	1:B:109:ASN:HD21	1.55	0.71
1:B:131:GLU:HG2	1:B:132:GLU:N	2.02	0.71
1:B:481:ARG:NH1	4:B:701:HOH:O	2.25	0.69
1:A:424:GLN:NE2	1:A:474:PRO:HD3	2.08	0.69
1:A:147:SER:O	1:A:389:PHE:HB3	1.92	0.69
1:A:94:ASN:HD22	1:A:103:ARG:NH2	1.86	0.68
1:B:18:GLY:HA3	4:B:685:HOH:O	1.93	0.67
1:B:424:GLN:NE2	1:B:474:PRO:HD3	2.10	0.66
1:B:147:SER:O	1:B:148:ALA:HB3	1.95	0.66
1:A:367:THR:HG22	1:A:369:GLU:N	2.07	0.65
1:A:94:ASN:ND2	1:A:103:ARG:HH21	1.88	0.64
1:B:287:ILE:HD11	1:B:305:LEU:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ARG:HB3	1:A:530:ARG:NH2	2.13	0.64
1:A:469:PHE:O	4:A:679:HOH:O	2.14	0.63
1:B:51:ASN:O	1:B:86:GLN:HG3	1.99	0.63
1:A:166:HIS:CD2	1:A:168:SER:H	2.17	0.63
1:A:331:HIS:HB2	1:A:332:PRO:HD2	1.79	0.63
1:A:224:LEU:HD13	1:A:340:MET:HE3	1.80	0.62
1:A:354:HIS:HA	4:A:563:HOH:O	1.98	0.62
1:A:187:ARG:NH1	1:A:379:ASP:O	2.33	0.62
1:B:59:ASP:HB2	1:B:340:MET:CE	2.31	0.61
1:A:96:ALA:O	1:A:100:MET:HG3	2.01	0.60
1:A:508:LYS:HE3	1:A:514:VAL:HG21	1.82	0.60
1:A:51:ASN:O	1:A:86:GLN:HG3	2.01	0.60
1:A:220:TRP:O	1:A:339:PRO:HD2	2.03	0.59
1:B:337:ARG:O	1:B:339:PRO:HD3	2.02	0.59
1:B:116:ARG:NH1	4:B:602:HOH:O	2.33	0.59
1:B:173:ASP:OD2	1:B:177:ALA:HB3	2.03	0.59
1:A:318:LYS:O	1:A:320:PRO:HD3	2.04	0.58
1:B:172:THR:HA	1:B:177:ALA:O	2.03	0.58
1:B:24:GLN:HE21	1:B:434:LEU:HD11	1.69	0.57
1:B:166:HIS:HD2	1:B:168:SER:H	1.51	0.57
1:B:166:HIS:CD2	1:B:168:SER:H	2.23	0.57
1:A:180:GLY:CA	4:A:646:HOH:O	2.53	0.56
1:B:45:GLY:HA3	1:B:49:TYR:HB2	1.87	0.56
1:A:166:HIS:HD2	1:A:168:SER:H	1.54	0.56
1:A:116:ARG:HG2	1:A:402:ARG:HB2	1.89	0.55
1:A:507:THR:HG22	1:A:513:VAL:HG22	1.88	0.55
1:B:202:PRO:HG3	1:B:344:TYR:HA	1.88	0.54
1:B:165:PHE:HE2	1:B:170:TRP:CZ3	2.26	0.54
1:B:172:THR:HB	1:B:176:GLY:HA2	1.90	0.54
1:A:520:HIS:CD2	1:A:520:HIS:C	2.86	0.54
1:B:18:GLY:N	4:B:685:HOH:O	2.41	0.53
1:B:131:GLU:HG2	1:B:132:GLU:H	1.71	0.53
1:A:85:SER:OG	1:A:87:PRO:HD2	2.09	0.53
1:B:59:ASP:HB2	1:B:340:MET:HE3	1.91	0.53
1:B:187:ARG:NH1	1:B:379:ASP:O	2.39	0.53
1:B:265:THR:C	1:B:267:VAL:H	2.17	0.52
1:A:165:PHE:HD1	1:A:171:PRO:HD2	1.74	0.51
1:A:418:SER:HB2	1:A:516:ARG:NH1	2.25	0.51
1:A:215:GLN:HG2	4:A:610:HOH:O	2.11	0.50
2:B:551:FAD:C6	3:B:552:NAP:C2N	2.90	0.50
1:B:74:ILE:HG21	1:B:95:ARG:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASN:ND2	1:B:103:ARG:HH21	2.05	0.50
1:A:490:PHE:CE2	1:A:496:ALA:HA	2.48	0.49
1:A:508:LYS:HB3	1:A:509:PRO:HD2	1.95	0.48
1:A:458:LEU:C	1:A:458:LEU:HD13	2.38	0.48
1:B:440:GLY:HA2	1:B:520:HIS:CD2	2.48	0.48
1:A:379:ASP:O	1:A:380:LEU:HD23	2.13	0.48
1:B:53:TYR:HB2	1:B:54:PRO:HD2	1.97	0.47
1:A:147:SER:O	1:A:147:SER:OG	2.30	0.47
1:B:295:LEU:HD11	1:B:305:LEU:HD23	1.97	0.47
1:B:515:ARG:O	1:B:516:ARG:HG2	2.14	0.47
1:B:129:ASP:C	1:B:130[A]:ASN:OD1	2.59	0.46
1:B:220:TRP:O	1:B:339:PRO:HD2	2.16	0.46
1:A:12:ALA:O	1:A:35:VAL:HA	2.16	0.46
1:A:13:VAL:HA	1:A:36:LEU:O	2.16	0.46
1:A:255:PHE:CE1	1:A:285:TYR:HD2	2.34	0.46
1:B:147:SER:O	1:B:148:ALA:CB	2.62	0.46
1:A:331:HIS:HB2	1:A:332:PRO:CD	2.46	0.45
1:B:490:PHE:CE1	1:B:517:THR:HG23	2.51	0.45
1:A:324:GLU:O	1:A:329:LYS:NZ	2.49	0.45
1:B:332:PRO:HG2	1:B:335:ALA:HB2	1.98	0.45
1:A:224:LEU:HD12	1:A:340:MET:HE3	1.95	0.45
1:B:502:TRP:CD1	1:B:503:VAL:HG23	2.51	0.45
1:A:263:LYS:HD3	1:A:293:ARG:HH12	1.82	0.44
1:A:217:THR:OG1	3:A:552:NAP:O2X	2.35	0.44
1:B:146:LEU:HA	1:B:146:LEU:HD23	1.76	0.44
1:B:515:ARG:C	1:B:516:ARG:CG	2.91	0.43
1:A:54:PRO:HG3	1:A:181:VAL:HG12	2.00	0.43
1:B:426:ARG:HH11	1:B:426:ARG:HG3	1.83	0.43
1:A:285:TYR:O	1:A:286:GLY:C	2.60	0.43
1:B:421:LEU:HA	1:B:482:TRP:CE2	2.52	0.43
1:A:45:GLY:HA2	1:A:93:VAL:HG11	2.00	0.43
1:A:13:VAL:HG22	1:A:36:LEU:HB3	2.00	0.43
1:B:62:SER:HB3	1:B:79:TRP:CD2	2.54	0.43
1:B:423:LEU:O	1:B:432:PHE:HA	2.18	0.43
1:B:220:TRP:CD1	1:B:333:PHE:HA	2.54	0.42
1:A:17:ALA:HB2	1:A:106:TYR:CE2	2.55	0.42
1:B:357:ASP:OD1	1:B:357:ASP:C	2.63	0.42
1:B:369:GLU:HB2	4:B:704:HOH:O	2.18	0.42
1:A:149:SER:HB3	1:A:168:SER:HG	1.75	0.42
1:B:94:ASN:HD22	1:B:103:ARG:NH2	2.07	0.42
1:B:123:LEU:HD12	1:B:123:LEU:C	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:HG2	1:A:109:ASN:HD21	1.84	0.42
1:B:53:TYR:CZ	1:B:196:THR:HG23	2.55	0.42
1:B:67:TYR:CE2	1:B:71:LYS:HG3	2.55	0.42
1:A:342:THR:HB	4:A:577:HOH:O	2.18	0.41
1:B:165:PHE:HE2	1:B:170:TRP:CE3	2.37	0.41
1:A:426:ARG:NH1	1:A:474:PRO:O	2.50	0.41
1:B:218:PRO:O	1:B:328:PRO:HG3	2.21	0.41
1:A:166:HIS:HD2	1:A:168:SER:OG	2.04	0.41
1:B:173:ASP:HB2	1:B:174:ALA:H	1.67	0.41
1:B:347:THR:HG22	1:B:353:VAL:HG21	2.02	0.41
1:A:79:TRP:O	1:A:229:MET:HG2	2.20	0.41
1:A:267:VAL:HG23	1:A:272:ARG:HG2	2.01	0.41
1:A:195:ALA:HA	1:A:339:PRO:HB3	2.02	0.41
1:A:389:PHE:N	1:A:389:PHE:CD2	2.89	0.41
1:A:530:ARG:HB3	1:A:530:ARG:HH21	1.83	0.41
1:A:324:GLU:HG3	1:A:329:LYS:NZ	2.36	0.41
1:A:154:ILE:HD13	1:A:154:ILE:HA	1.81	0.40
1:A:185:GLY:HA2	1:A:209:LYS:HB2	2.04	0.40
1:A:119:GLU:HG2	4:A:567:HOH:O	2.21	0.40
1:A:165:PHE:CD1	1:A:171:PRO:HD2	2.54	0.40
1:A:163:GLU:HB2	1:A:382:VAL:HG22	2.03	0.40
1:B:390:ASP:HB3	1:B:394:GLY:HA3	2.03	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	534/545 (98%)	511 (96%)	21 (4%)	2 (0%)	30	37
1	B	530/545 (97%)	498 (94%)	30 (6%)	2 (0%)	30	37
All	All	1064/1090 (98%)	1009 (95%)	51 (5%)	4 (0%)	30	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
1	A	435	VAL
1	B	148	ALA
1	B	445	ASN

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	446/454 (98%)	420 (94%)	26 (6%)	18	27
1	B	442/454 (97%)	415 (94%)	27 (6%)	17	24
All	All	888/908 (98%)	835 (94%)	53 (6%)	18	26

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	13	VAL
1	A	34	LYS
1	A	119	GLU
1	A	131	GLU
1	A	154	ILE
1	A	164	SER
1	A	196	THR
1	A	215	GLN
1	A	216	ARG
1	A	217	THR
1	A	259	ARG
1	A	263	LYS
1	A	273	ASP
1	A	296	LEU
1	A	330	ASP
1	A	359	ARG
1	A	363	ILE
1	A	367	THR

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Mol	Chain	Res	Type
1	A	389	PHE
1	A	444	CYS
1	A	458	LEU
1	A	465	LYS
1	A	495	LEU
1	A	507	THR
1	A	520	HIS
1	B	74	ILE
1	B	102	VAL
1	B	122	ARG
1	B	130[A]	ASN
1	B	130[B]	ASN
1	B	131	GLU
1	B	147	SER
1	B	149	SER
1	B	150	ARG
1	B	273	ASP
1	B	285	TYR
1	B	287	ILE
1	B	293	ARG
1	B	296	LEU
1	B	325	LYS
1	B	369	GLU
1	B	372	LYS
1	B	390	ASP
1	B	435	VAL
1	B	441	SER
1	B	444	CYS
1	B	465	LYS
1	B	471	TYR
1	B	499	ASN
1	B	504	LYS
1	B	517	THR
1	B	543	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	51	ASN
1	A	82	ASN
1	A	94	ASN

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Mol	Chain	Res	Type
1	A	109	ASN
1	A	166	HIS
1	A	354	HIS
1	A	406	ASN
1	A	424	GLN
1	A	499	ASN
1	A	540	ASN
1	B	24	GLN
1	B	82	ASN
1	B	94	ASN
1	B	105	HIS
1	B	109	ASN
1	B	166	HIS
1	B	219	ASN
1	B	424	GLN
1	B	467	ASN
1	B	480	ASN
1	B	520	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAP	A	552	-	50,52,52	2.36	9 (18%)	71,80,80	1.69	13 (18%)
2	FAD	A	551	-	58,58,58	1.34	5 (8%)	85,89,89	1.79	15 (17%)
2	FAD	B	551	-	58,58,58	1.26	6 (10%)	85,89,89	1.73	17 (20%)
3	NAP	B	552	-	50,52,52	1.99	10 (20%)	71,80,80	1.93	16 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	552	-	-	12/35/67/67	0/5/5/5
2	FAD	A	551	-	-	4/34/50/50	0/6/6/6
2	FAD	B	551	-	-	6/34/50/50	0/6/6/6
3	NAP	B	552	-	-	0/35/67/67	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	552	NAP	O7N-C7N	11.60	1.45	1.24
3	B	552	NAP	O7N-C7N	8.88	1.40	1.24
3	A	552	NAP	PA-O3	5.83	1.65	1.59
2	A	551	FAD	C4X-N5	4.88	1.41	1.30
3	A	552	NAP	C2N-N1N	4.49	1.39	1.35
3	B	552	NAP	C2N-N1N	4.46	1.39	1.35
2	B	551	FAD	C4X-N5	4.31	1.40	1.30
3	A	552	NAP	PN-O3	4.10	1.63	1.59
3	A	552	NAP	C2A-N3A	4.07	1.41	1.33
3	B	552	NAP	O4D-C1D	3.92	1.46	1.40
2	A	551	FAD	C2A-N1A	3.34	1.39	1.33
3	A	552	NAP	C2A-N1A	3.34	1.39	1.33
3	B	552	NAP	PA-O3	3.24	1.63	1.59
2	A	551	FAD	PA-O3P	3.22	1.63	1.59
2	A	551	FAD	C2A-N3A	3.13	1.39	1.33
2	B	551	FAD	C2A-N1A	3.08	1.39	1.33
3	B	552	NAP	C2A-N3A	3.04	1.39	1.33
3	B	552	NAP	PN-O3	2.83	1.62	1.59
2	A	551	FAD	C10-N1	2.63	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	551	FAD	C10-N1	2.60	1.38	1.33
3	A	552	NAP	C8A-N7A	2.50	1.36	1.31
3	A	552	NAP	O4D-C1D	2.49	1.44	1.40
3	B	552	NAP	C5N-C4N	2.49	1.43	1.38
3	B	552	NAP	C2A-N1A	2.45	1.38	1.33
2	B	551	FAD	O4'-C4'	-2.42	1.38	1.43
2	B	551	FAD	C1'-N10	2.23	1.53	1.47
3	B	552	NAP	C6N-N1N	2.08	1.40	1.35
3	A	552	NAP	C6A-N1A	2.08	1.41	1.35
3	B	552	NAP	P2B-O2B	2.07	1.63	1.59
2	B	551	FAD	P-O3P	2.05	1.61	1.59

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	551	FAD	N3A-C2A-N1A	-6.73	118.39	128.58
3	B	552	NAP	C4D-O4D-C1D	-6.06	104.38	109.92
3	B	552	NAP	C3N-C7N-N7N	5.21	124.16	117.74
3	A	552	NAP	C5A-C4A-N3A	-5.18	119.58	126.72
2	B	551	FAD	N3A-C2A-N1A	-5.17	120.75	128.58
3	B	552	NAP	C5A-C4A-N3A	-4.90	119.97	126.72
2	A	551	FAD	O4B-C1B-N9A	4.52	116.77	108.09
3	A	552	NAP	N3A-C2A-N1A	-4.31	122.05	128.58
2	B	551	FAD	C5A-C4A-N3A	-4.20	120.93	126.72
3	A	552	NAP	C5A-N7A-C8A	4.17	110.00	103.45
2	A	551	FAD	C5A-C4A-N3A	-4.16	120.98	126.72
3	A	552	NAP	C3N-C7N-N7N	-4.11	112.68	117.74
3	B	552	NAP	O7N-C7N-C3N	-4.10	114.58	119.60
2	B	551	FAD	C4-N3-C2	-4.03	118.48	125.64
3	A	552	NAP	C4A-C5A-N7A	-3.90	106.12	110.58
3	B	552	NAP	N3A-C2A-N1A	-3.88	122.70	128.58
2	B	551	FAD	C4-C4X-N5	3.79	123.44	118.21
2	B	551	FAD	N9A-C8A-N7A	-3.76	108.60	113.94
2	A	551	FAD	C2A-N3A-C4A	3.74	120.96	111.83
3	A	552	NAP	N9A-C8A-N7A	-3.69	108.71	113.94
3	B	552	NAP	N9A-C8A-N7A	-3.62	108.80	113.94
2	A	551	FAD	O3B-C3B-C4B	-3.59	100.78	111.08
3	B	552	NAP	C5A-N7A-C8A	3.56	109.05	103.45
2	A	551	FAD	N9A-C8A-N7A	-3.53	108.92	113.94
3	B	552	NAP	C2B-C1B-N9A	-3.51	107.97	113.75
3	B	552	NAP	C2A-N3A-C4A	3.44	120.23	111.83
2	B	551	FAD	N3A-C4A-N9A	3.43	133.00	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	552	NAP	C4A-C5A-N7A	-3.39	106.71	110.58
2	B	551	FAD	C4X-C4-N3	3.36	121.80	113.25
2	A	551	FAD	C4-N3-C2	-3.35	119.69	125.64
2	A	551	FAD	C4X-C4-N3	3.35	121.77	113.25
3	A	552	NAP	C2A-N3A-C4A	3.33	119.96	111.83
2	A	551	FAD	C4-C4X-N5	3.29	122.75	118.21
2	B	551	FAD	C4X-C10-N10	3.26	121.15	116.48
2	B	551	FAD	C5A-N7A-C8A	3.25	108.56	103.45
2	B	551	FAD	C10-C4X-N5	-3.22	118.23	124.81
2	A	551	FAD	C10-N1-C2	3.17	123.71	116.85
2	B	551	FAD	O3B-C3B-C4B	-3.16	102.00	111.08
3	A	552	NAP	N3A-C4A-N9A	3.01	132.29	127.17
2	A	551	FAD	C4X-C10-N10	3.00	120.78	116.48
2	A	551	FAD	C10-C4X-N5	-2.98	118.72	124.81
2	B	551	FAD	C2A-N3A-C4A	2.98	119.10	111.83
3	B	552	NAP	O2N-PN-O3	2.88	115.06	107.27
2	A	551	FAD	C4X-C10-N1	-2.86	117.58	124.59
2	B	551	FAD	C10-N1-C2	2.83	122.97	116.85
2	A	551	FAD	N3A-C4A-N9A	2.79	131.91	127.17
2	A	551	FAD	C5A-N7A-C8A	2.77	107.80	103.45
3	B	552	NAP	N3A-C4A-N9A	2.73	131.81	127.17
3	B	552	NAP	O4B-C1B-N9A	2.65	113.19	108.09
3	A	552	NAP	C2B-C1B-N9A	2.65	118.11	113.75
3	A	552	NAP	C6A-C5A-C4A	2.57	120.68	117.18
2	B	551	FAD	C4A-N9A-C8A	2.53	108.39	105.74
2	B	551	FAD	C4X-C10-N1	-2.52	118.41	124.59
3	A	552	NAP	O7N-C7N-C3N	2.39	122.52	119.60
2	B	551	FAD	O4'-C4'-C3'	-2.37	103.71	109.25
3	B	552	NAP	C5B-C4B-C3B	-2.28	107.02	115.21
3	B	552	NAP	C5N-C6N-N1N	-2.25	117.32	120.38
3	B	552	NAP	C5A-C4A-N9A	2.20	108.21	105.81
3	A	552	NAP	C5A-C4A-N9A	2.12	108.12	105.81
3	A	552	NAP	C2N-C3N-C4N	2.10	120.71	118.26
2	B	551	FAD	C5'-C4'-C3'	2.00	116.00	112.22

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	551	FAD	N10-C1'-C2'-O2'
2	A	551	FAD	N10-C1'-C2'-C3'
2	B	551	FAD	N10-C1'-C2'-O2'

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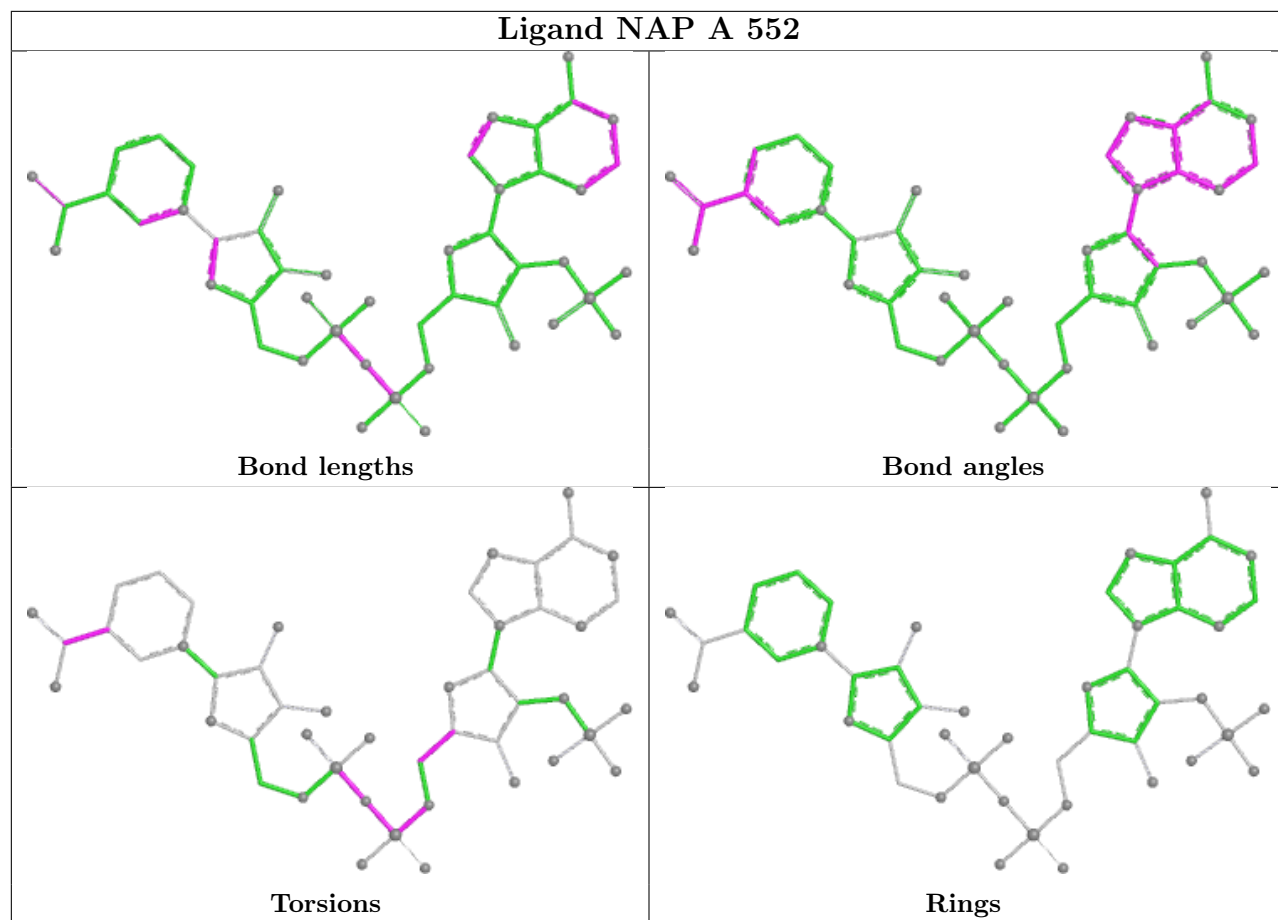
Mol	Chain	Res	Type	Atoms
2	B	551	FAD	N10-C1'-C2'-C3'
2	B	551	FAD	PA-O3P-P-O5'
3	A	552	NAP	C2N-C3N-C7N-O7N
3	A	552	NAP	C2N-C3N-C7N-N7N
3	A	552	NAP	C4N-C3N-C7N-O7N
3	A	552	NAP	C4N-C3N-C7N-N7N
3	A	552	NAP	O4B-C4B-C5B-O5B
3	A	552	NAP	C3B-C4B-C5B-O5B
2	A	551	FAD	O4B-C4B-C5B-O5B
3	A	552	NAP	PA-O3-PN-O5D
3	A	552	NAP	PN-O3-PA-O2A
3	A	552	NAP	C5B-O5B-PA-O1A
3	A	552	NAP	C5B-O5B-PA-O2A
3	A	552	NAP	C5B-O5B-PA-O3
2	B	551	FAD	P-O3P-PA-O1A
2	A	551	FAD	C3B-C4B-C5B-O5B
2	B	551	FAD	P-O3P-PA-O2A
2	B	551	FAD	O4B-C4B-C5B-O5B
3	A	552	NAP	PN-O3-PA-O1A

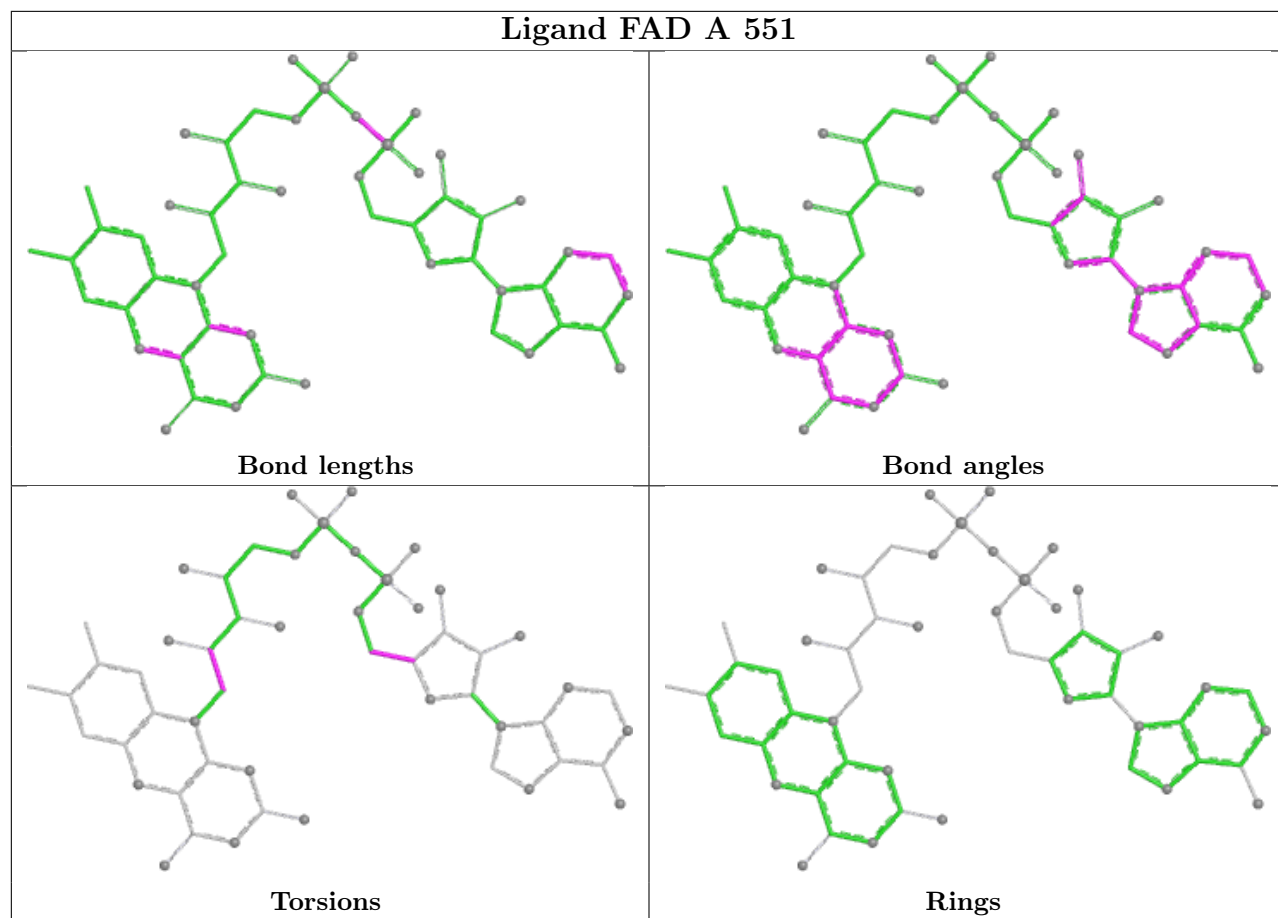
There are no ring outliers.

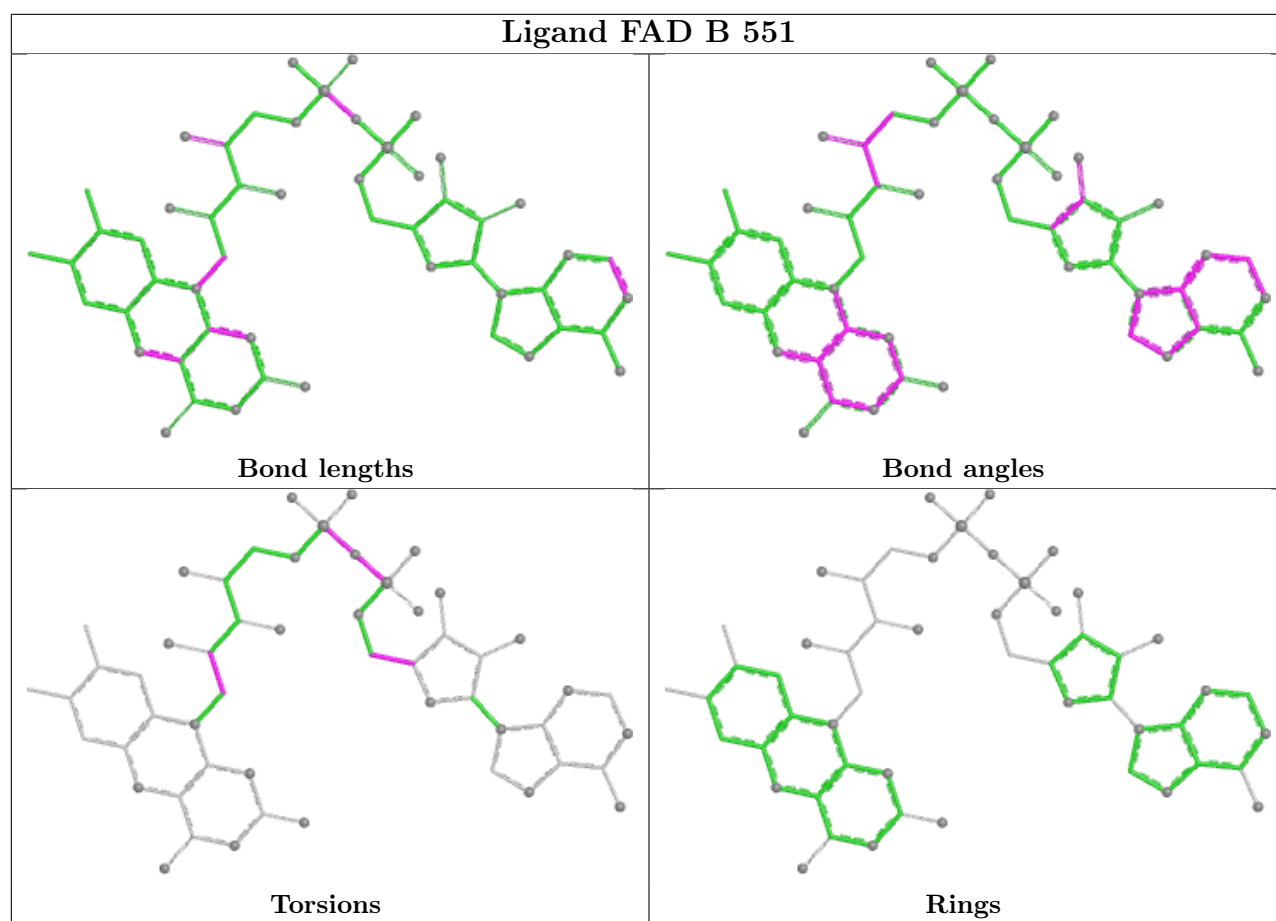
3 monomers are involved in 4 short contacts:

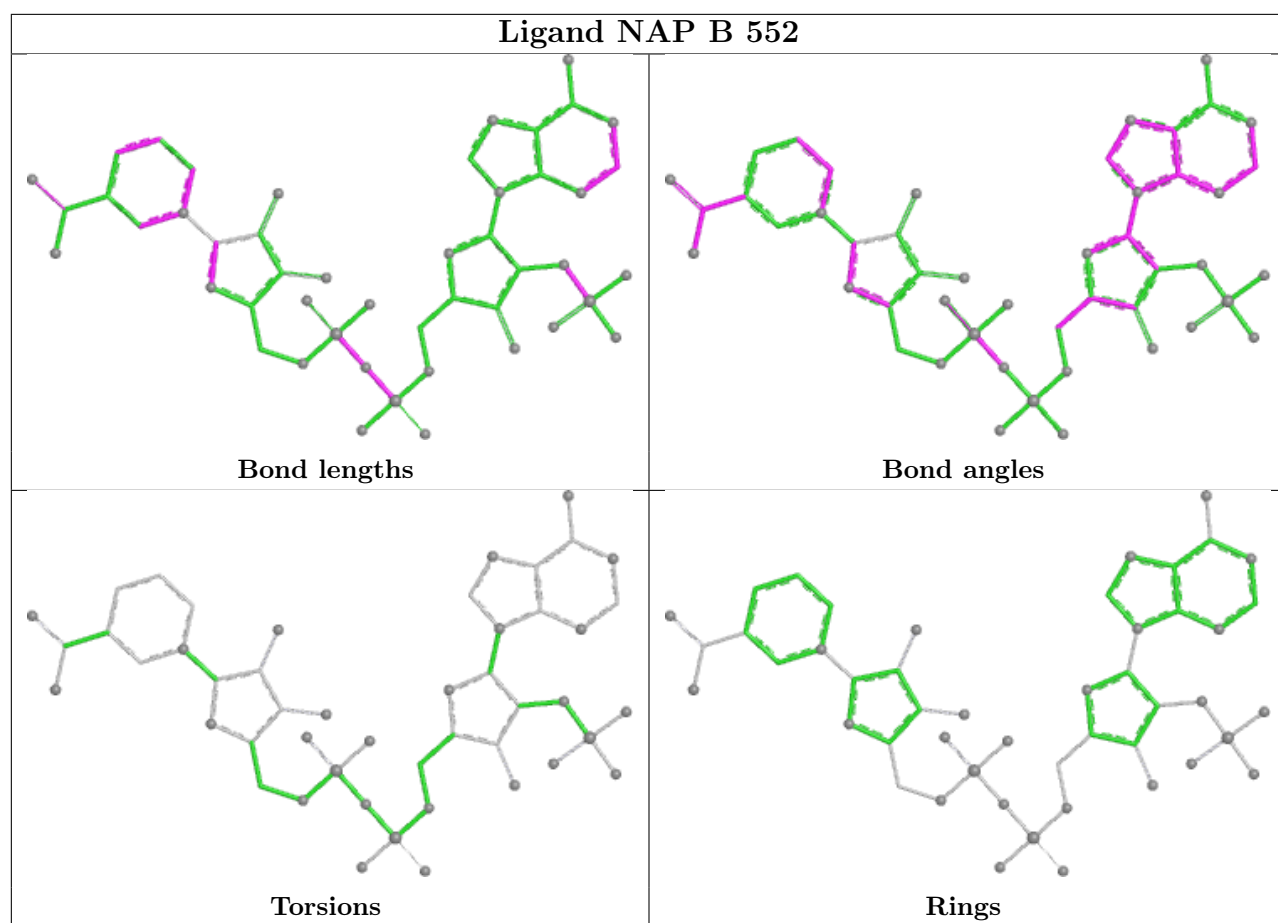
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	552	NAP	1	0
2	B	551	FAD	2	0
3	B	552	NAP	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	537/545 (98%)	-0.35	6 (1%)	78 79	11, 27, 41, 52	1 (0%)
1	B	532/545 (97%)	-0.46	3 (0%)	85 87	11, 23, 35, 44	2 (0%)
All	All	1069/1090 (98%)	-0.41	9 (0%)	82 83	11, 25, 39, 52	3 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	PRO	3.7
1	A	150	ARG	3.1
1	A	130	ASN	2.4
1	A	501	TRP	2.4
1	B	180	GLY	2.3
1	B	175	GLU	2.3
1	B	506	THR	2.1
1	A	512	SER	2.1
1	A	389	PHE	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.

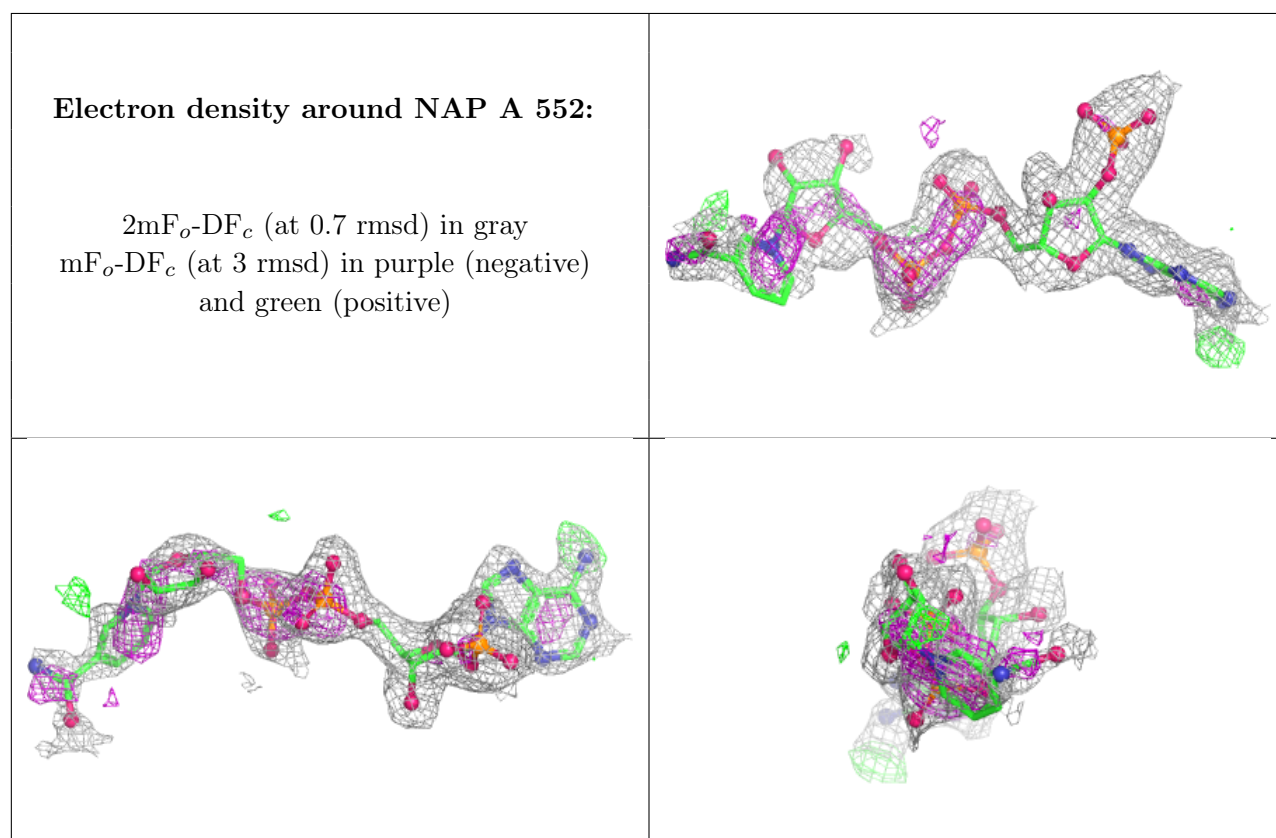
6.4 Ligands [i](#)

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.

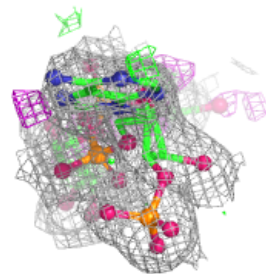
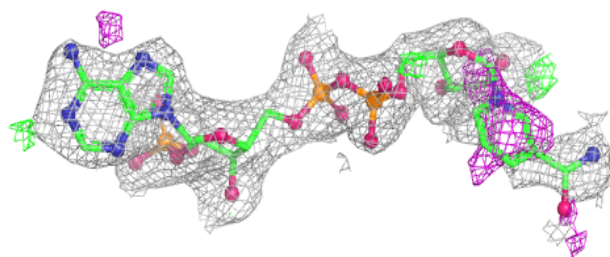
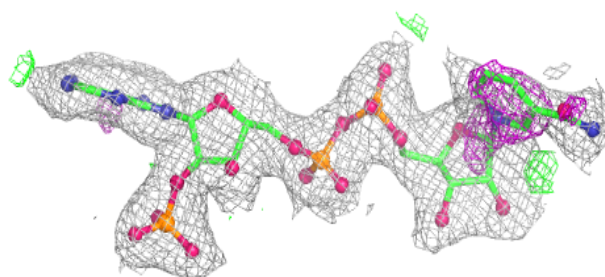
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	A	552	48/48	0.86	0.12	32,39,49,50	0
3	NAP	B	552	48/48	0.95	0.08	16,23,36,41	0
2	FAD	A	551	53/53	0.97	0.06	16,23,27,29	0
2	FAD	B	551	53/53	0.98	0.05	10,16,21,22	0

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.

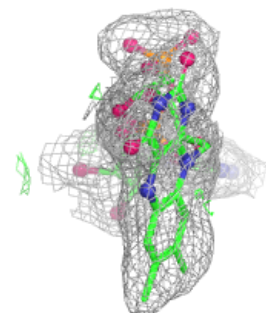
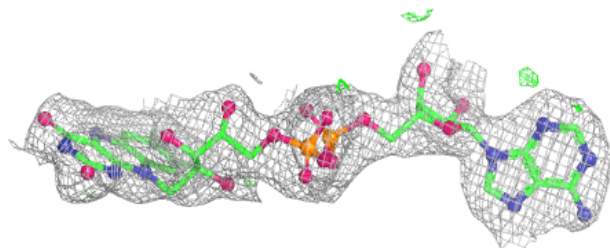
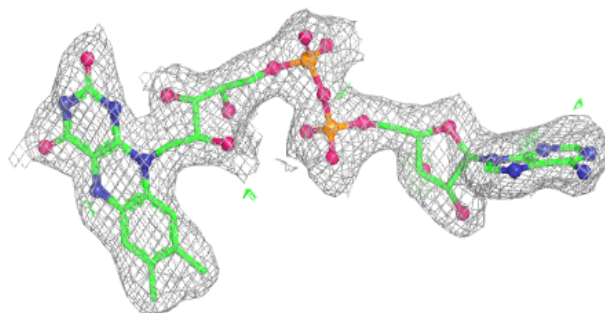


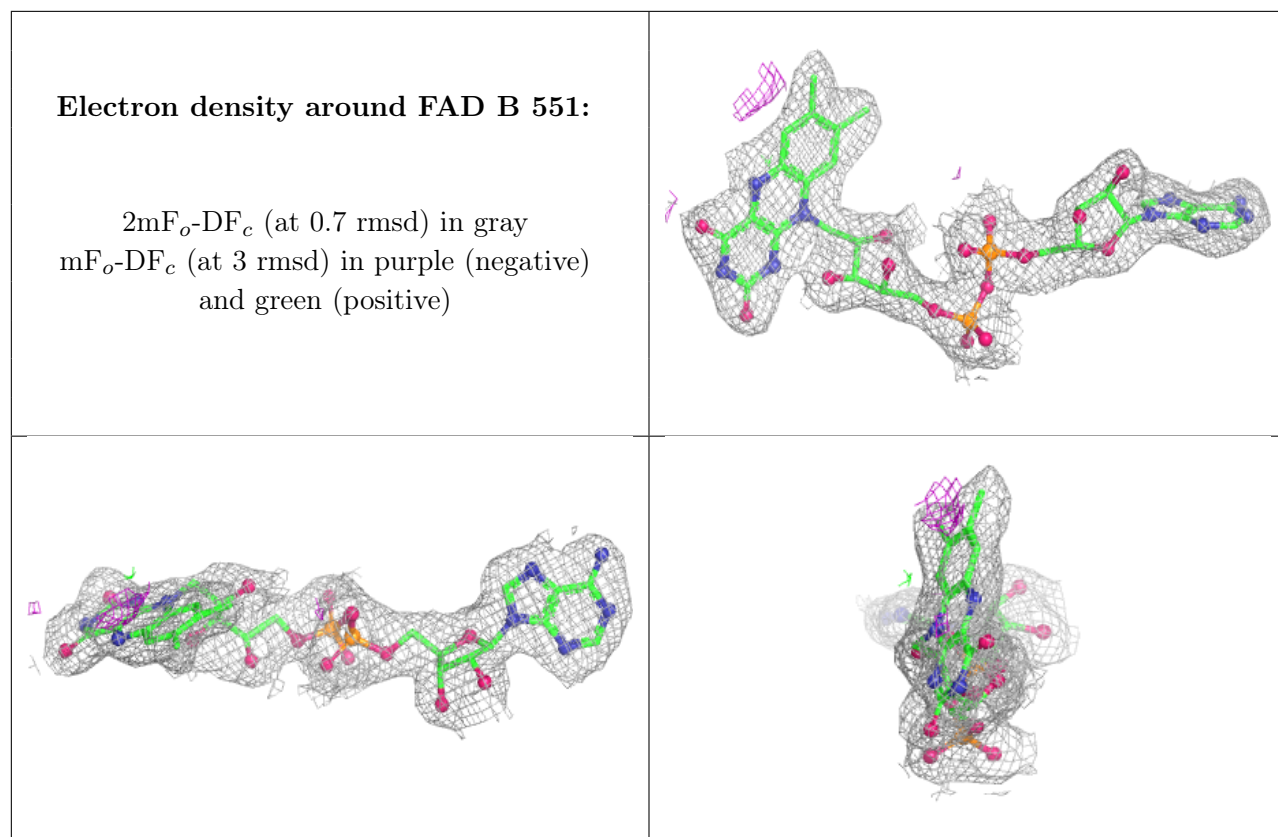
Electron density around NAP B 552:

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

**Electron density around FAD A 551:**

$2mF_o-DF_c$ (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.