



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:30 AM UTC

PDB ID : 6JYG / pdb_00006jyg
Title : Crystal Structure of L-threonine dehydrogenase from *Phytophthora infestans*
Authors : Yoneda, K.; Sakuraba, H.; Ohshima, T.
Deposited on : 2019-04-26
Resolution : 2.31 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:

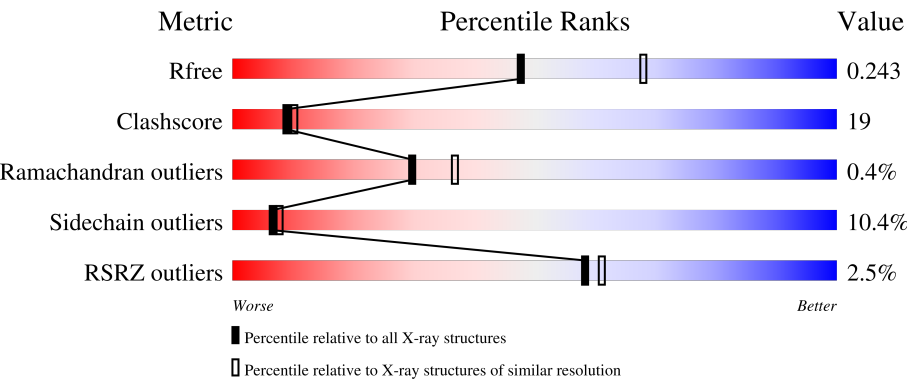
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	345	51%28%8%11%
1	B	345	3%46%34%8%11%
1	C	345	2%48%32%8%11%
1	D	345	3%57%24%8%11%
1	E	345	2%52%27%7%12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	345	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	A	401	-	X	-	-
3	PE8	A	402	-	-	X	-
3	PE8	D	402	-	-	X	-

2 Entry composition [i](#)

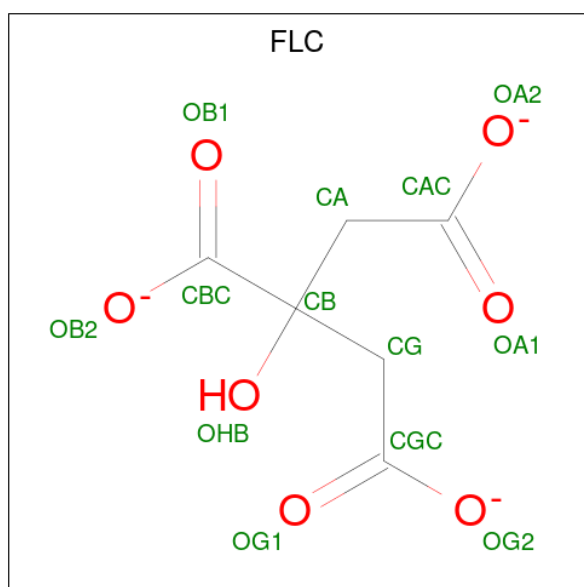
There are 5 unique types of molecules in this entry. The entry contains 15108 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-threonine 3-dehydrogenase, putative.

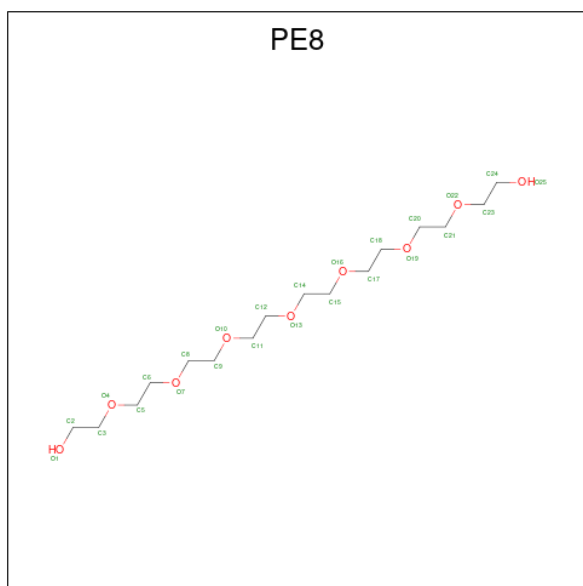
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2395	1518	397	462	18			
1	B	306	Total	C	N	O	S	0	0	0
			2395	1518	397	462	18			
1	C	306	Total	C	N	O	S	0	0	0
			2395	1518	397	462	18			
1	D	307	Total	C	N	O	S	0	0	0
			2406	1524	401	463	18			
1	E	304	Total	C	N	O	S	0	0	0
			2378	1506	394	460	18			
1	F	307	Total	C	N	O	S	0	0	0
			2406	1524	401	463	18			

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



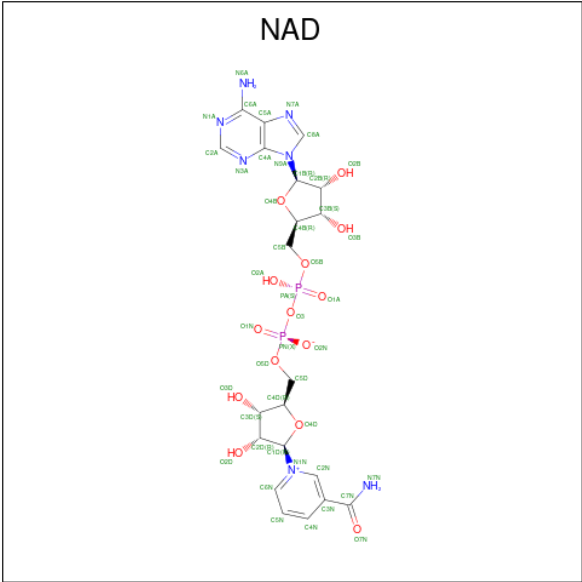
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: $C_{16}H_{34}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	16	9		
3	D	1	Total	C	O	0	0
			25	16	9		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

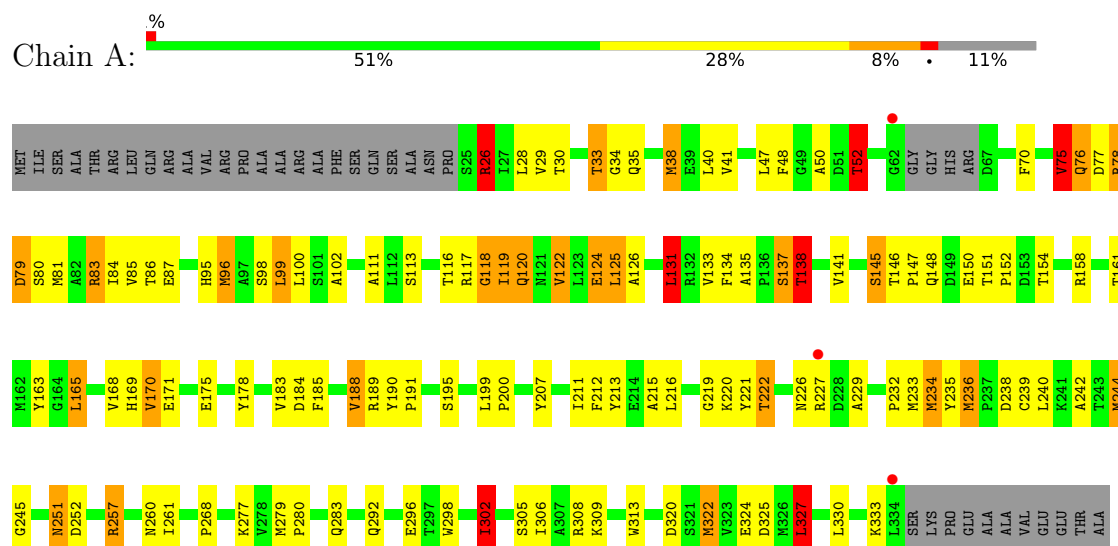
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	56	Total	O	0	0
			56	56		
5	C	58	Total	O	0	0
			58	58		
5	D	46	Total	O	0	0
			46	46		
5	E	58	Total	O	0	0
			58	58		
5	F	54	Total	O	0	0
			54	54		

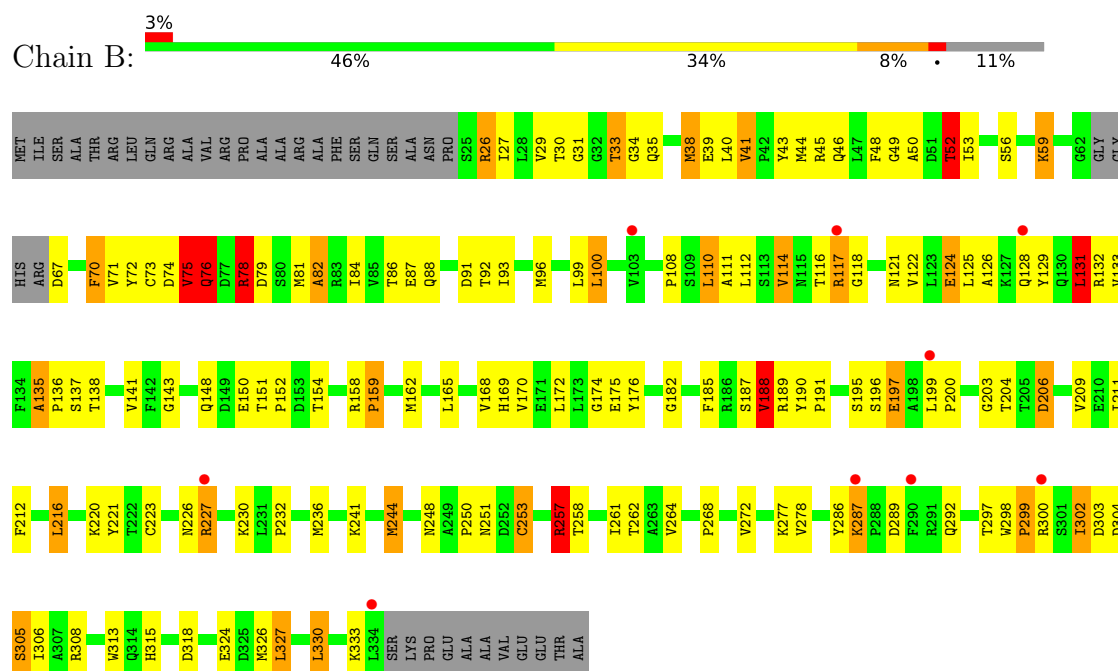
3 Residue-property plots

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.

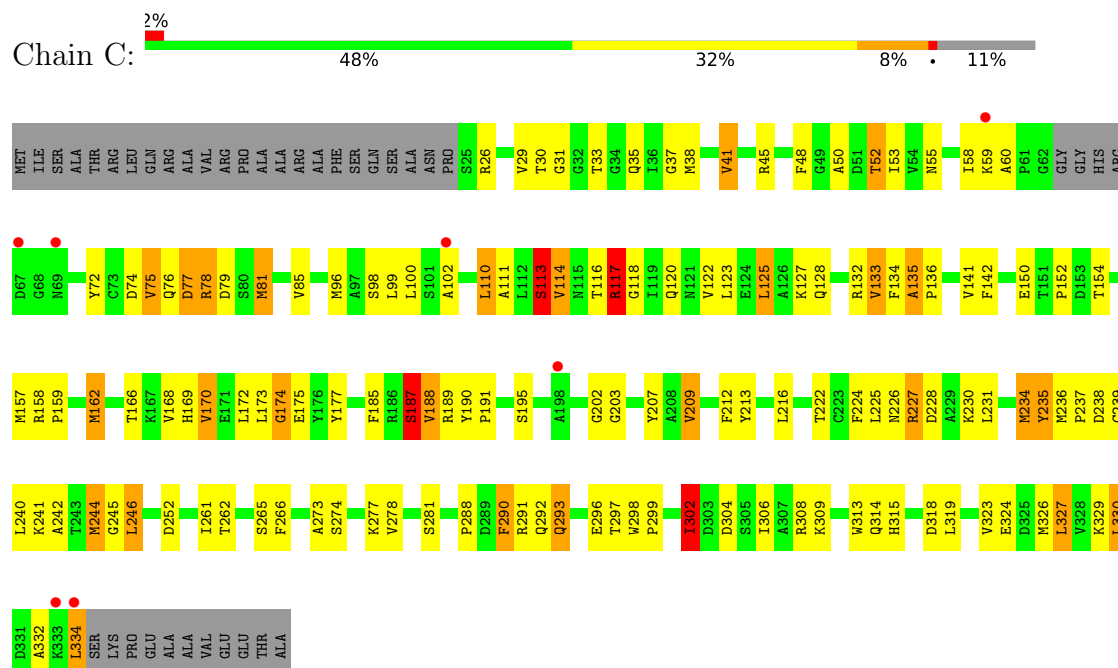
• Molecule 1: L-threonine 3-dehydrogenase, putative



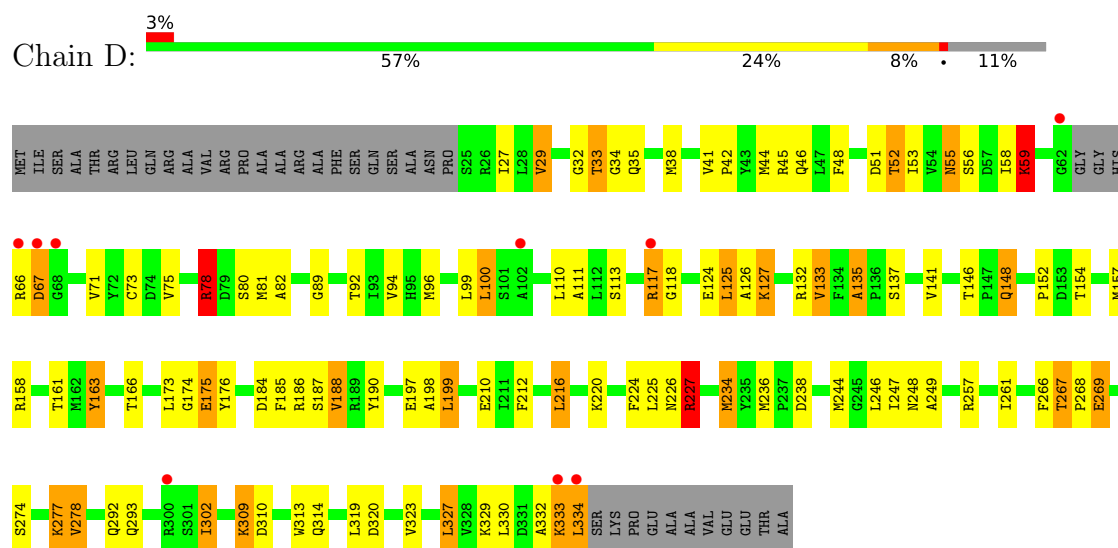
• Molecule 1: L-threonine 3-dehydrogenase, putative



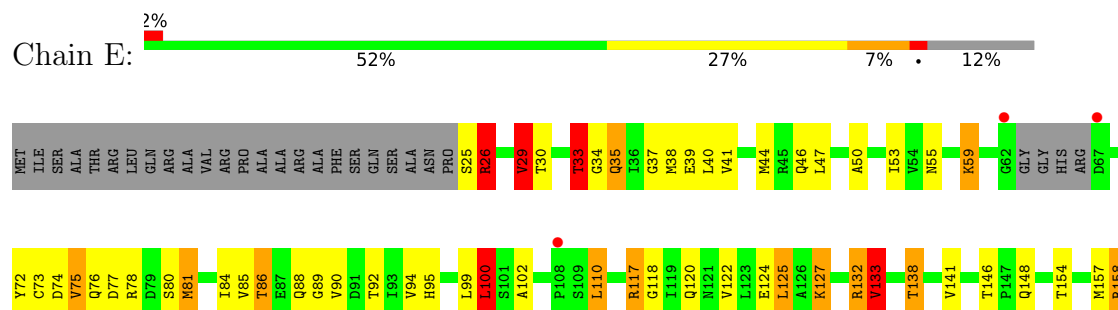
- Molecule 1: L-threonine 3-dehydrogenase, putative

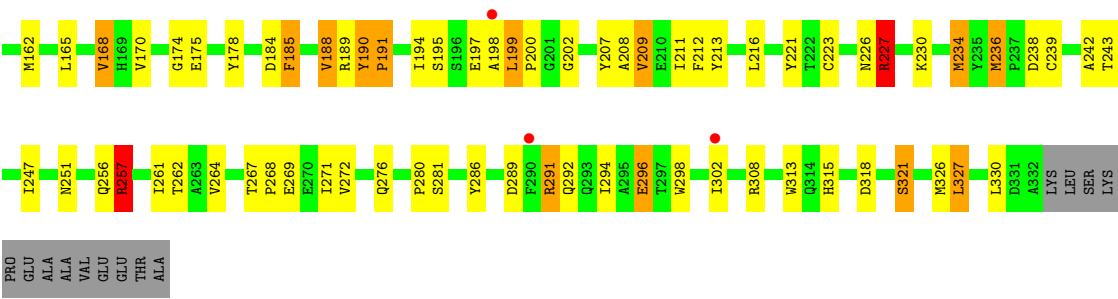


- Molecule 1: L-threonine 3-dehydrogenase, putative

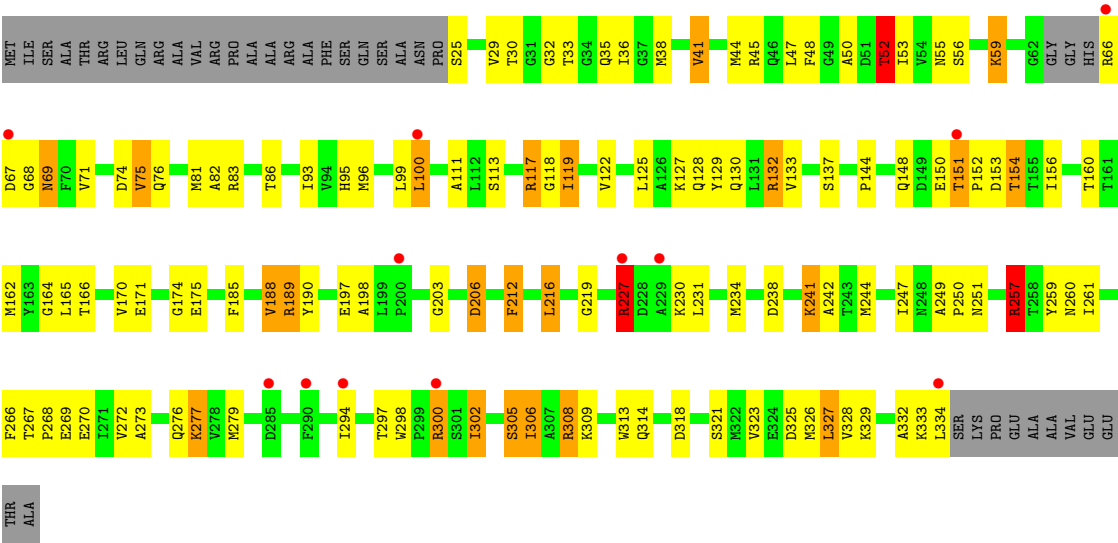


- Molecule 1: L-threonine 3-dehydrogenase, putative





● Molecule 1: L-threonine 3-dehydrogenase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	171.21Å 98.86Å 152.51Å 90.00° 106.72° 90.00°	Depositor
Resolution (Å)	49.28 – 2.31 49.28 – 2.31	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.28-2.31) 93.1 (49.28-2.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.32Å)	Xtrriage
Refinement program	REFMAC, CNS 1.3	Depositor
R, R_{free}	0.238 , 0.242 0.239 , 0.243	Depositor DCC
R_{free} test set	5028 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtrriage
Anisotropy	0.159	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15108	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3805e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FLC, NAD, PE8

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	1.69	34/2446 (1.4%)	1.66	37/3322 (1.1%)
1	B	1.71	35/2446 (1.4%)	1.66	40/3322 (1.2%)
1	C	1.68	27/2446 (1.1%)	1.61	30/3322 (0.9%)
1	D	1.54	20/2457 (0.8%)	1.58	28/3336 (0.8%)
1	E	1.64	25/2429 (1.0%)	1.63	33/3300 (1.0%)
1	F	1.55	12/2457 (0.5%)	1.61	33/3336 (1.0%)
All	All	1.64	153/14681 (1.0%)	1.63	201/19938 (1.0%)

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	VAL	CA-CB	10.72	1.60	1.54
1	A	41	VAL	CA-C	10.08	1.62	1.52
1	C	162	MET	C-O	9.83	1.35	1.24
1	C	113	SER	CA-C	8.78	1.63	1.52
1	B	138	THR	C-O	8.72	1.35	1.23
1	B	302	ILE	C-O	8.54	1.33	1.24
1	B	121	ASN	C-O	-8.40	1.14	1.24
1	B	289	ASP	CA-C	8.02	1.61	1.53
1	B	258	THR	CA-C	7.78	1.62	1.52
1	B	174	GLY	N-CA	7.76	1.55	1.45
1	E	41	VAL	CA-C	7.48	1.60	1.52
1	A	161	THR	C-O	7.47	1.32	1.23
1	A	152	PRO	C-O	7.45	1.32	1.23
1	C	102	ALA	N-CA	7.39	1.55	1.46
1	B	172	LEU	C-O	7.34	1.32	1.24
1	B	299	PRO	CA-C	7.24	1.61	1.52
1	D	234	MET	CA-C	-7.22	1.43	1.52
1	A	302	ILE	C-O	7.16	1.31	1.24
1	D	188	VAL	C-O	7.12	1.31	1.24
1	D	175	GLU	N-CA	7.11	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	83	ARG	CZ-NH1	7.08	1.42	1.32
1	B	41	VAL	CA-C	7.01	1.59	1.52
1	E	191	PRO	CA-C	7.00	1.62	1.52
1	A	188	VAL	C-O	6.80	1.30	1.24
1	A	80	SER	CA-C	6.74	1.61	1.52
1	A	76	GLN	CA-C	6.71	1.62	1.52
1	C	152	PRO	C-O	6.68	1.32	1.23
1	D	110	LEU	C-O	-6.65	1.16	1.24
1	B	159	PRO	C-O	6.61	1.31	1.23
1	E	73	CYS	C-O	-6.56	1.16	1.23
1	C	170	VAL	CA-CB	-6.44	1.47	1.54
1	E	102	ALA	N-CA	6.43	1.53	1.46
1	C	158	ARG	C-O	-6.37	1.17	1.24
1	A	131	LEU	C-O	6.37	1.31	1.23
1	C	77	ASP	CA-C	6.37	1.60	1.53
1	B	188	VAL	N-CA	-6.21	1.39	1.46
1	C	170	VAL	CA-C	6.18	1.60	1.52
1	A	207	TYR	N-CA	6.17	1.53	1.46
1	F	302	ILE	C-O	6.17	1.30	1.24
1	D	247	ILE	CA-CB	6.16	1.60	1.54
1	F	308	ARG	N-CA	6.15	1.53	1.46
1	E	138	THR	N-CA	-6.14	1.38	1.46
1	B	302	ILE	CA-CB	6.09	1.61	1.54
1	B	297	THR	N-CA	6.05	1.54	1.46
1	A	236	MET	N-CA	6.01	1.52	1.46
1	C	100	LEU	N-CA	6.00	1.53	1.45
1	A	236	MET	C-O	-5.99	1.18	1.24
1	A	245	GLY	CA-C	5.97	1.58	1.52
1	C	273	ALA	N-CA	-5.97	1.38	1.46
1	E	125	LEU	C-O	-5.97	1.17	1.24
1	F	82	ALA	N-CA	5.94	1.53	1.46
1	B	84	ILE	CA-CB	5.92	1.60	1.54
1	E	80	SER	N-CA	5.91	1.53	1.46
1	C	141	VAL	CA-C	5.91	1.61	1.52
1	B	169	HIS	C-O	5.89	1.31	1.24
1	A	86	THR	CB-CG2	-5.87	1.33	1.52
1	D	186	ARG	CA-C	-5.86	1.45	1.52
1	C	173	LEU	CA-C	5.85	1.60	1.52
1	B	176	TYR	CA-C	5.82	1.60	1.52
1	B	82	ALA	CA-C	5.82	1.60	1.52
1	B	93	ILE	CA-CB	5.80	1.61	1.54
1	F	305	SER	C-O	5.78	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	98	SER	C-O	-5.78	1.17	1.23
1	B	191	PRO	CA-C	5.76	1.60	1.52
1	E	72	TYR	C-O	-5.76	1.17	1.24
1	C	304	ASP	CA-C	5.75	1.60	1.53
1	D	302	ILE	CA-CB	5.72	1.61	1.54
1	F	93	ILE	CA-CB	5.71	1.61	1.54
1	A	170	VAL	N-CA	5.70	1.53	1.46
1	C	141	VAL	C-O	5.68	1.31	1.24
1	D	148	GLN	CA-C	5.66	1.60	1.52
1	B	135	ALA	CA-C	5.65	1.57	1.52
1	B	304	ASP	C-O	5.63	1.31	1.24
1	C	159	PRO	C-O	5.63	1.30	1.23
1	C	191	PRO	C-O	-5.63	1.16	1.24
1	A	138	THR	N-CA	-5.62	1.39	1.46
1	C	245	GLY	C-O	5.57	1.30	1.23
1	D	55	ASN	CA-C	5.57	1.59	1.52
1	D	82	ALA	CA-C	5.55	1.60	1.52
1	B	114	VAL	CA-CB	5.53	1.61	1.54
1	A	85	VAL	N-CA	5.52	1.53	1.46
1	A	28	LEU	CA-C	-5.52	1.46	1.52
1	E	39	GLU	N-CA	5.51	1.53	1.46
1	E	162	MET	C-O	5.50	1.30	1.24
1	E	100	LEU	N-CA	5.47	1.52	1.45
1	A	158	ARG	CZ-NH2	5.47	1.40	1.33
1	A	102	ALA	N-CA	5.46	1.53	1.46
1	B	306	ILE	N-CA	-5.45	1.39	1.46
1	D	29	VAL	CA-CB	5.45	1.61	1.54
1	D	176	TYR	C-O	-5.45	1.17	1.24
1	F	127	LYS	N-CA	-5.45	1.39	1.46
1	D	78	ARG	CA-C	5.45	1.60	1.52
1	E	294	ILE	CA-C	5.43	1.59	1.52
1	B	72	TYR	N-CA	-5.42	1.39	1.46
1	E	84	ILE	CA-C	5.42	1.59	1.52
1	D	274	SER	CA-C	5.41	1.59	1.52
1	A	52	THR	N-CA	-5.38	1.39	1.46
1	C	306	ILE	N-CA	5.37	1.52	1.46
1	C	114	VAL	CA-CB	5.36	1.60	1.54
1	C	58	ILE	CA-CB	5.36	1.61	1.54
1	A	191	PRO	CA-C	5.36	1.60	1.52
1	B	289	ASP	N-CA	5.34	1.52	1.46
1	B	299	PRO	C-O	5.33	1.30	1.23
1	A	77	ASP	C-O	5.30	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	CYS	C-O	-5.29	1.17	1.24
1	B	287	LYS	CA-C	5.28	1.59	1.52
1	F	41	VAL	CA-C	5.28	1.58	1.52
1	B	87	GLU	C-O	-5.26	1.17	1.24
1	B	100	LEU	N-CA	5.26	1.53	1.45
1	D	236	MET	CA-C	5.26	1.58	1.52
1	C	37	GLY	C-O	5.25	1.30	1.23
1	E	184	ASP	N-CA	-5.25	1.39	1.46
1	B	170	VAL	CA-CB	-5.24	1.48	1.54
1	F	59	LYS	C-O	-5.24	1.17	1.24
1	F	188	VAL	N-CA	-5.24	1.40	1.46
1	C	302	ILE	CA-CB	5.20	1.61	1.54
1	E	33	THR	CA-CB	5.20	1.62	1.53
1	A	26	ARG	CA-C	5.20	1.59	1.52
1	A	124	GLU	C-O	-5.19	1.17	1.24
1	A	327	LEU	N-CA	-5.17	1.40	1.46
1	A	169	HIS	CA-C	5.17	1.59	1.52
1	E	271	ILE	C-O	5.16	1.30	1.24
1	A	122	VAL	N-CA	5.16	1.53	1.46
1	C	41	VAL	CA-CB	-5.15	1.51	1.54
1	B	76	GLN	C-O	-5.14	1.17	1.24
1	B	159	PRO	N-CA	5.14	1.53	1.47
1	B	75	VAL	CA-C	5.13	1.58	1.52
1	A	305	SER	CA-C	5.13	1.59	1.52
1	D	89	GLY	N-CA	5.12	1.53	1.45
1	B	117	ARG	CA-C	5.12	1.59	1.52
1	D	246	LEU	N-CA	5.12	1.52	1.46
1	E	89	GLY	C-O	-5.11	1.18	1.24
1	D	274	SER	C-O	5.10	1.29	1.24
1	E	127	LYS	CA-C	5.09	1.59	1.52
1	D	59	LYS	N-CA	5.08	1.52	1.45
1	C	127	LYS	CA-C	5.08	1.59	1.52
1	A	98	SER	C-O	-5.07	1.17	1.23
1	E	77	ASP	C-O	5.07	1.30	1.23
1	E	53	ILE	CA-CB	5.06	1.60	1.54
1	F	189	ARG	N-CA	5.05	1.53	1.46
1	A	171	GLU	N-CA	5.05	1.52	1.46
1	A	147	PRO	C-O	5.04	1.29	1.23
1	A	325	ASP	C-O	-5.04	1.18	1.24
1	E	236	MET	CA-CB	5.04	1.58	1.54
1	E	59	LYS	N-CA	5.04	1.51	1.45
1	E	185	PHE	C-O	-5.04	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	281	SER	N-CA	-5.03	1.39	1.46
1	A	163	TYR	C-O	5.03	1.29	1.24
1	D	80	SER	CA-C	5.03	1.59	1.52
1	F	36	ILE	C-O	5.02	1.30	1.24
1	E	209	VAL	C-O	5.02	1.28	1.23
1	C	187	SER	C-O	5.01	1.30	1.23
1	C	278	VAL	C-O	-5.01	1.18	1.23

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	ILE	N-CA-C	-10.99	102.37	113.47
1	A	168	VAL	N-CA-C	-10.48	100.13	110.72
1	A	146	THR	CA-C-N	-9.29	110.15	119.90
1	A	146	THR	C-N-CA	-9.29	110.15	119.90
1	A	306	ILE	N-CA-C	8.88	119.68	110.36
1	E	202	GLY	N-CA-C	8.40	125.84	114.92
1	C	135	ALA	CA-C-N	8.30	128.81	119.93
1	C	135	ALA	C-N-CA	8.30	128.81	119.93
1	D	29	VAL	CB-CA-C	8.24	121.13	110.91
1	B	158	ARG	CA-C-N	-8.16	111.61	119.85
1	B	158	ARG	C-N-CA	-8.16	111.61	119.85
1	B	78	ARG	N-CA-C	8.13	120.14	111.28
1	C	174	GLY	N-CA-C	-8.03	103.09	112.73
1	A	79	ASP	N-CA-C	7.98	120.06	111.36
1	C	209	VAL	CB-CA-C	7.79	120.99	111.80
1	F	257	ARG	CD-NE-CZ	7.78	135.29	124.40
1	D	248	ASN	N-CA-C	7.74	122.30	113.01
1	E	26	ARG	CG-CD-NE	7.58	128.68	112.00
1	E	190	TYR	N-CA-C	7.53	118.83	109.57
1	C	319	LEU	N-CA-C	7.50	120.10	111.11
1	D	267	THR	CA-C-N	-7.46	110.77	119.05
1	D	267	THR	C-N-CA	-7.46	110.77	119.05
1	A	154	THR	CB-CA-C	7.44	122.72	110.74
1	C	81	MET	CG-SD-CE	-7.12	85.23	100.90
1	C	168	VAL	N-CA-C	-7.10	103.27	111.00
1	A	134	PHE	N-CA-C	-7.07	97.37	108.90
1	B	168	VAL	N-CA-C	-7.01	103.64	110.72
1	B	50	ALA	N-CA-C	-7.00	104.38	113.12
1	E	158	ARG	CA-C-N	-6.88	113.56	120.31
1	E	158	ARG	C-N-CA	-6.88	113.56	120.31
1	E	37	GLY	N-CA-C	6.79	120.86	112.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	197	GLU	N-CA-C	6.78	121.69	113.41
1	B	287	LYS	CB-CA-C	6.75	117.67	110.65
1	A	50	ALA	N-CA-C	-6.72	103.20	111.33
1	D	146	THR	CA-C-N	-6.71	112.84	119.76
1	D	146	THR	C-N-CA	-6.71	112.84	119.76
1	F	127	LYS	N-CA-C	6.68	118.22	111.07
1	B	154	THR	CB-CA-C	6.67	121.67	110.79
1	F	59	LYS	CD-CE-NZ	6.61	133.05	111.90
1	B	143	GLY	CA-C-N	6.57	126.51	119.28
1	B	143	GLY	C-N-CA	6.57	126.51	119.28
1	F	154	THR	CB-CA-C	6.57	121.32	110.74
1	C	278	VAL	CB-CA-C	-6.56	105.00	111.30
1	E	29	VAL	CB-CA-C	6.56	119.76	110.84
1	A	222	THR	CB-CA-C	6.53	121.44	110.79
1	E	298	TRP	CA-C-N	-6.53	113.26	119.85
1	E	298	TRP	C-N-CA	-6.53	113.26	119.85
1	F	231	LEU	CA-C-N	-6.35	113.14	119.99
1	F	231	LEU	C-N-CA	-6.35	113.14	119.99
1	A	151	THR	CA-C-N	6.33	126.30	120.03
1	A	151	THR	C-N-CA	6.33	126.30	120.03
1	A	79	ASP	N-CA-CB	6.30	119.49	110.16
1	F	298	TRP	N-CA-C	6.30	118.80	110.36
1	C	114	VAL	CG1-CB-CG2	-6.26	97.03	110.80
1	C	117	ARG	CA-CB-CG	6.24	126.58	114.10
1	E	165	LEU	N-CA-C	-6.23	104.59	111.82
1	F	212	PHE	N-CA-C	6.23	117.87	111.14
1	B	197	GLU	CA-C-N	6.21	129.54	120.71
1	B	197	GLU	C-N-CA	6.21	129.54	120.71
1	A	135	ALA	CA-C-N	-6.15	113.96	120.66
1	A	135	ALA	C-N-CA	-6.15	113.96	120.66
1	C	235	TYR	N-CA-C	-6.15	101.38	110.48
1	B	110	LEU	N-CA-C	-6.13	104.14	111.69
1	F	151	THR	CA-C-N	6.13	126.10	120.03
1	F	151	THR	C-N-CA	6.13	126.10	120.03
1	C	240	LEU	N-CA-C	-6.09	104.56	111.14
1	E	55	ASN	N-CA-C	-6.08	99.36	109.46
1	A	119	ILE	N-CA-CB	6.08	117.66	110.55
1	E	208	ALA	CA-C-N	-6.07	115.19	122.35
1	E	208	ALA	C-N-CA	-6.07	115.19	122.35
1	B	298	TRP	CA-C-N	-6.06	113.54	119.78
1	B	298	TRP	C-N-CA	-6.06	113.54	119.78
1	C	117	ARG	N-CA-CB	6.04	119.10	110.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	GLY	N-CA-C	-6.04	105.04	112.77
1	A	199	LEU	N-CA-C	-6.03	101.76	110.08
1	C	298	TRP	N-CA-C	6.02	118.29	110.40
1	B	26	ARG	N-CA-C	5.99	119.31	109.72
1	F	308	ARG	N-CA-C	-5.97	104.46	110.97
1	C	79	ASP	N-CA-C	5.96	119.82	112.54
1	C	244	MET	N-CA-C	5.95	118.24	111.11
1	F	257	ARG	NE-CZ-NH2	-5.93	113.86	119.20
1	E	81	MET	N-CA-C	5.90	117.71	111.28
1	E	59	LYS	CA-CB-CG	5.84	125.79	114.10
1	B	298	TRP	N-CA-C	5.83	117.31	110.31
1	D	174	GLY	N-CA-C	-5.83	105.30	112.77
1	E	59	LYS	CB-CA-C	-5.83	98.70	109.37
1	B	206	ASP	N-CA-C	5.82	119.90	112.34
1	D	94	VAL	CB-CA-C	5.79	119.63	112.45
1	B	38	MET	N-CA-C	-5.78	105.49	112.54
1	B	148	GLN	N-CA-C	5.78	120.33	113.16
1	C	177	TYR	N-CA-C	5.77	118.31	111.33
1	E	33	THR	CB-CA-C	5.74	119.87	110.17
1	F	219	GLY	N-CA-C	-5.73	107.34	115.43
1	F	306	ILE	N-CA-C	5.73	116.38	110.36
1	F	153	ASP	CA-C-N	-5.72	114.72	123.07
1	F	153	ASP	C-N-CA	-5.72	114.72	123.07
1	E	50	ALA	N-CA-C	-5.72	105.05	111.28
1	F	148	GLN	N-CA-C	5.71	120.25	113.28
1	C	209	VAL	CG1-CB-CG2	-5.71	98.24	110.80
1	E	133	VAL	N-CA-C	5.70	116.49	108.17
1	A	96	MET	N-CA-C	-5.70	106.50	113.50
1	B	257	ARG	CD-NE-CZ	5.70	132.37	124.40
1	C	213	TYR	N-CA-C	-5.68	105.17	111.36
1	A	26	ARG	N-CA-C	5.66	119.28	110.17
1	B	244	MET	CG-SD-CE	-5.66	88.45	100.90
1	B	220	LYS	N-CA-C	5.65	117.43	108.79
1	F	249	ALA	CA-C-N	-5.64	113.90	119.99
1	F	249	ALA	C-N-CA	-5.64	113.90	119.99
1	D	135	ALA	CA-C-N	-5.61	113.44	120.51
1	D	135	ALA	C-N-CA	-5.61	113.44	120.51
1	D	126	ALA	N-CA-C	5.61	118.11	111.33
1	B	114	VAL	N-CA-CB	5.59	118.15	110.54
1	A	298	TRP	N-CA-C	5.58	117.72	110.40
1	B	258	THR	N-CA-C	5.58	118.34	109.24
1	C	110	LEU	N-CA-C	-5.58	104.70	112.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	166	THR	CB-CA-C	-5.55	100.35	110.63
1	B	52	THR	N-CA-C	5.55	119.67	113.01
1	E	236	MET	CA-C-N	-5.55	113.31	119.19
1	E	236	MET	C-N-CA	-5.55	113.31	119.19
1	C	266	PHE	N-CA-C	5.51	117.22	108.79
1	B	131	LEU	CA-CB-CG	5.50	135.57	116.30
1	A	84	ILE	N-CA-C	-5.45	105.40	110.53
1	D	148	GLN	N-CA-CB	-5.45	101.94	110.44
1	C	31	GLY	N-CA-C	-5.44	105.45	114.48
1	F	52	THR	N-CA-C	5.42	119.88	113.16
1	E	168	VAL	N-CA-C	-5.40	104.34	111.09
1	C	53	ILE	CG1-CB-CG2	-5.40	94.51	110.70
1	D	249	ALA	CA-C-N	-5.40	114.20	119.76
1	D	249	ALA	C-N-CA	-5.40	114.20	119.76
1	E	257	ARG	CD-NE-CZ	5.39	131.95	124.40
1	A	99	LEU	N-CA-C	-5.37	102.57	110.52
1	E	46	GLN	CB-CA-C	-5.35	101.91	110.79
1	A	38	MET	CB-CG-SD	-5.34	96.67	112.70
1	A	83	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	E	296	GLU	N-CA-C	5.32	118.56	111.75
1	D	163	TYR	CA-C-N	-5.31	114.08	119.98
1	D	163	TYR	C-N-CA	-5.31	114.08	119.98
1	B	70	PHE	N-CA-C	5.30	117.61	109.07
1	B	31	GLY	N-CA-C	-5.30	105.68	114.48
1	B	124	GLU	CB-CA-C	5.30	119.86	110.85
1	C	154	THR	CB-CA-C	5.29	119.41	110.79
1	A	137	SER	N-CA-C	-5.29	101.83	109.29
1	E	154	THR	CB-CA-C	5.28	119.24	110.74
1	B	182	GLY	CA-C-N	-5.27	113.27	121.18
1	B	182	GLY	C-N-CA	-5.27	113.27	121.18
1	F	75	VAL	N-CA-C	-5.26	104.67	112.04
1	F	132	ARG	CB-CG-CD	-5.26	99.19	111.30
1	A	120	GLN	N-CA-C	5.26	117.42	111.11
1	D	216	LEU	N-CA-C	5.25	117.09	111.36
1	C	187	SER	CA-CB-OG	-5.25	100.61	111.10
1	A	251	ASN	N-CA-C	5.24	117.67	111.33
1	A	148	GLN	N-CA-C	5.23	119.66	113.28
1	E	75	VAL	N-CA-CB	-5.23	98.89	111.23
1	E	190	TYR	CA-C-O	5.22	124.10	119.71
1	F	197	GLU	CA-CB-CG	-5.22	103.66	114.10
1	F	257	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	D	96	MET	N-CA-C	-5.21	106.93	113.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	294	ILE	CA-C-N	5.21	128.63	120.82
1	F	294	ILE	C-N-CA	5.21	128.63	120.82
1	B	230	LYS	N-CA-C	-5.20	101.49	109.76
1	A	145	SER	CB-CA-C	-5.20	99.13	109.99
1	C	278	VAL	N-CA-C	-5.20	107.69	111.90
1	A	183	VAL	N-CA-CB	5.19	116.77	110.95
1	A	118	GLY	N-CA-C	-5.18	106.14	112.77
1	F	160	THR	CA-C-N	-5.17	113.82	122.92
1	F	160	THR	C-N-CA	-5.17	113.82	122.92
1	D	277	LYS	N-CA-CB	5.16	117.70	110.12
1	E	47	LEU	N-CA-C	5.16	116.98	111.36
1	A	75	VAL	CG1-CB-CG2	5.16	122.14	110.80
1	E	257	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	F	137	SER	N-CA-C	-5.15	102.03	109.29
1	C	60	ALA	CA-C-N	5.14	125.14	119.90
1	C	60	ALA	C-N-CA	5.14	125.14	119.90
1	B	162	MET	N-CA-C	-5.13	105.58	111.07
1	F	227	ARG	N-CA-C	5.13	118.31	111.75
1	A	33	THR	N-CA-C	-5.12	105.93	113.61
1	B	188	VAL	N-CA-C	-5.11	100.89	108.45
1	B	204	THR	N-CA-C	-5.11	105.35	112.45
1	D	161	THR	CA-C-N	5.11	127.44	120.54
1	D	161	THR	C-N-CA	5.11	127.44	120.54
1	D	197	GLU	N-CA-C	5.09	119.49	113.12
1	D	269	GLU	N-CA-C	5.07	117.54	111.71
1	D	152	PRO	CA-C-N	5.07	127.49	120.29
1	D	152	PRO	C-N-CA	5.07	127.49	120.29
1	E	170	VAL	N-CA-C	5.06	115.68	110.36
1	B	128	GLN	N-CA-CB	5.06	117.47	109.94
1	F	164	GLY	N-CA-C	5.05	118.36	112.50
1	B	248	ASN	CA-C-N	-5.05	113.00	120.68
1	B	248	ASN	C-N-CA	-5.05	113.00	120.68
1	E	110	LEU	N-CA-C	-5.05	105.47	111.69
1	A	244	MET	CG-SD-CE	-5.05	89.80	100.90
1	A	80	SER	N-CA-C	-5.04	105.78	111.28
1	F	216	LEU	N-CA-C	5.03	116.77	111.28
1	A	85	VAL	CA-C-N	5.03	127.02	120.28
1	A	85	VAL	C-N-CA	5.03	127.02	120.28
1	C	72	TYR	CA-C-N	-5.02	115.73	122.86
1	C	72	TYR	C-N-CA	-5.02	115.73	122.86
1	D	133	VAL	N-CA-C	5.02	115.94	108.46
1	A	165	LEU	N-CA-C	-5.01	105.90	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	MET	CB-CA-C	5.00	120.77	110.31
1	E	197	GLU	N-CA-C	5.00	118.79	111.04

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	2395	0	2352	88	0
1	B	2395	0	2352	84	0
1	C	2395	0	2352	107	0
1	D	2406	0	2365	85	0
1	E	2378	0	2328	95	0
1	F	2406	0	2365	90	0
2	A	13	0	5	3	0
2	B	13	0	5	3	0
2	C	13	0	5	1	0
2	D	13	0	5	1	0
2	E	26	0	10	4	0
2	F	13	0	5	3	0
3	A	25	0	34	13	0
3	D	25	0	34	10	0
4	A	44	0	26	5	0
4	B	44	0	26	7	0
4	C	44	0	26	4	0
4	D	44	0	26	4	0
4	E	44	0	26	6	0
4	F	44	0	26	8	0
5	A	56	0	0	5	0
5	B	56	0	0	3	0
5	C	58	0	0	8	0
5	D	46	0	0	0	0
5	E	58	0	0	4	0
5	F	54	0	0	5	0
All	All	15108	0	14373	540	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 19.

All (540) 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:E:234:MET:HE2	1:E:239:CYS:HA	1.22	1.17
1:C:227:ARG:H	1:C:227:ARG:CD	1.55	1.15
1:D:277:LYS:HB2	3:D:402:PE8:H232	1.30	1.10
1:A:234:MET:HE2	1:A:239:CYS:HA	1.31	1.07
1:C:227:ARG:H	1:C:227:ARG:HD2	0.93	1.05
1:C:227:ARG:HD2	1:C:227:ARG:N	1.71	1.04
1:D:117:ARG:HG2	1:D:117:ARG:HH11	1.20	1.02
1:B:135:ALA:O	1:B:187:SER:HB3	1.59	1.02
1:D:78:ARG:HH11	1:D:78:ARG:HG2	1.25	1.00
1:B:308:ARG:HH22	1:B:315:HIS:HD2	1.07	0.99
1:C:81:MET:HE1	1:C:122:VAL:HG22	1.44	0.98
1:A:292:GLN:O	1:A:296:GLU:HG3	1.63	0.98
1:B:326:MET:HA	5:B:531:HOH:O	1.64	0.97
1:A:277:LYS:HB2	3:A:402:PE8:H22	1.47	0.96
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.29	0.95
1:B:100:LEU:HD13	2:B:401:FLC:HA2	1.46	0.95
1:C:117:ARG:HH22	1:E:120:GLN:HE22	1.15	0.91
1:E:227:ARG:H	1:E:227:ARG:HD2	1.36	0.90
1:B:308:ARG:HH22	1:B:315:HIS:CD2	1.89	0.90
1:E:234:MET:HE2	1:E:239:CYS:CA	2.01	0.90
1:B:78:ARG:HH21	1:B:124:GLU:HG2	1.36	0.89
1:E:195:SER:HB2	5:E:515:HOH:O	1.72	0.89
1:C:120:GLN:HE22	1:E:117:ARG:HH22	1.19	0.89
1:A:234:MET:HE2	1:A:239:CYS:CA	2.02	0.88
1:A:277:LYS:NZ	3:A:402:PE8:H122	1.88	0.87
1:F:81:MET:HE1	1:F:122:VAL:HG22	1.59	0.85
1:F:75:VAL:HG12	1:F:118:GLY:CA	2.06	0.84
1:D:75:VAL:HA	1:D:81:MET:HE1	1.58	0.84
1:A:78:ARG:HD2	1:A:125:LEU:HD13	1.60	0.83
1:C:116:THR:O	1:C:120:GLN:HG3	1.78	0.83
1:F:44:MET:HG2	1:F:244:MET:CE	2.08	0.83
1:D:75:VAL:HG12	1:D:118:GLY:HA2	1.58	0.82
1:E:226:ASN:H	1:E:292:GLN:NE2	1.78	0.82
1:B:35:GLN:HE22	4:B:402:NAD:H72N	1.29	0.81
1:F:75:VAL:HG12	1:F:118:GLY:HA2	1.63	0.81
1:E:190:TYR:HB2	4:E:403:NAD:C5N	2.11	0.81
1:F:44:MET:HG2	1:F:244:MET:HE2	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:THR:HG21	1:E:59:LYS:HB2	1.62	0.81
1:C:308:ARG:HH21	1:C:315:HIS:HD2	1.30	0.79
1:B:303:ASP:OD1	1:B:305:SER:HB2	1.83	0.79
1:C:135:ALA:O	1:C:187:SER:HB3	1.82	0.79
1:E:227:ARG:H	1:E:227:ARG:CD	1.96	0.79
1:A:324:GLU:HG2	3:A:402:PE8:H32	1.65	0.78
1:C:234:MET:HE2	1:C:238:ASP:C	2.08	0.78
1:E:74:ASP:OD1	1:E:76:GLN:HG2	1.83	0.78
1:D:277:LYS:HB2	3:D:402:PE8:C23	2.12	0.78
1:E:262:THR:HB	1:E:302:ILE:HG12	1.66	0.76
1:D:277:LYS:NZ	3:D:402:PE8:H171	2.01	0.76
1:A:200:PRO:HB2	5:A:525:HOH:O	1.85	0.76
1:A:126:ALA:HA	1:A:131:LEU:HB2	1.66	0.76
1:D:78:ARG:HH21	1:D:124:GLU:HG2	1.51	0.75
1:A:257:ARG:HG3	1:A:257:ARG:NH1	1.97	0.75
1:D:78:ARG:HH21	1:D:124:GLU:CG	1.99	0.75
1:F:318:ASP:HB3	5:F:537:HOH:O	1.84	0.75
1:C:308:ARG:NH2	1:C:315:HIS:HD2	1.84	0.75
1:D:227:ARG:O	1:D:269:GLU:HG2	1.86	0.74
1:A:35:GLN:NE2	4:A:403:NAD:H72N	1.84	0.74
1:D:135:ALA:O	1:D:187:SER:HB2	1.87	0.74
1:A:145:SER:HB2	5:A:534:HOH:O	1.86	0.74
1:B:135:ALA:O	1:B:187:SER:CB	2.36	0.74
1:C:117:ARG:HH21	1:E:117:ARG:HH21	1.36	0.73
1:F:45:ARG:HG2	1:F:50:ALA:HA	1.68	0.73
1:B:257:ARG:HH11	1:B:257:ARG:HG3	1.53	0.73
1:D:38:MET:HE1	1:D:198:ALA:HB2	1.70	0.72
1:D:277:LYS:CB	3:D:402:PE8:H232	2.13	0.72
1:B:251:ASN:OD1	1:B:257:ARG:NH2	2.23	0.72
1:D:226:ASN:H	1:D:292:GLN:NE2	1.87	0.72
1:D:277:LYS:HZ2	3:D:402:PE8:H171	1.52	0.72
1:B:308:ARG:NH2	1:B:315:HIS:HD2	1.86	0.72
1:F:29:VAL:HG11	1:F:41:VAL:HG22	1.72	0.71
1:B:92:THR:HG23	1:B:132:ARG:HG3	1.73	0.71
1:C:172:LEU:CD1	1:E:168:VAL:HG21	2.20	0.71
1:C:195:SER:HB3	1:C:236:MET:HB2	1.72	0.71
1:D:113:SER:O	1:D:117:ARG:HB2	1.90	0.71
1:B:141:VAL:O	1:B:159:PRO:HD3	1.91	0.71
1:F:325:ASP:OD1	1:F:329:LYS:HE2	1.91	0.70
1:C:99:LEU:HG	1:C:114:VAL:HG21	1.72	0.70
1:D:78:ARG:HG2	1:D:78:ARG:NH1	1.99	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:VAL:HG21	1:D:157:MET:HE2	1.72	0.70
1:C:274:SER:O	1:C:277:LYS:HB2	1.92	0.69
1:D:78:ARG:HD2	1:D:125:LEU:HD13	1.75	0.69
1:E:35:GLN:CG	1:E:198:ALA:HB3	2.21	0.69
1:B:190:TYR:HB2	4:B:402:NAD:C5N	2.23	0.68
1:C:188:VAL:HG11	1:C:261:ILE:HD13	1.74	0.68
1:C:308:ARG:NH2	1:C:315:HIS:CD2	2.62	0.68
1:B:91:ASP:HA	1:B:131:LEU:HD12	1.75	0.68
1:F:75:VAL:HG12	1:F:118:GLY:HA3	1.73	0.68
1:C:35:GLN:HA	1:C:38:MET:HE3	1.75	0.68
1:A:260:ASN:HB3	1:A:302:ILE:CD1	2.24	0.68
1:A:190:TYR:HB2	4:A:403:NAD:C5N	2.24	0.67
1:B:35:GLN:NE2	4:B:402:NAD:N7N	2.41	0.67
1:F:38:MET:HE3	5:F:531:HOH:O	1.94	0.67
1:B:44:MET:HB2	1:B:53:ILE:CD1	2.24	0.67
1:F:273:ALA:HA	1:F:276:GLN:HG2	1.77	0.67
1:F:53:ILE:N	1:F:53:ILE:HD12	2.09	0.67
1:B:44:MET:HB2	1:B:53:ILE:HD11	1.77	0.67
1:D:333:LYS:O	1:D:334:LEU:HD23	1.94	0.67
1:A:251:ASN:OD1	1:A:257:ARG:NH2	2.29	0.66
1:C:157:MET:HE1	1:C:189:ARG:HH21	1.60	0.66
1:E:35:GLN:HG2	1:E:198:ALA:HB3	1.77	0.66
1:B:200:PRO:HB3	1:B:209:VAL:HG23	1.77	0.66
1:A:116:THR:O	1:A:120:GLN:HG3	1.94	0.65
1:C:308:ARG:HH21	1:C:315:HIS:CD2	2.14	0.65
1:E:100:LEU:HD12	2:E:401:FLC:HA2	1.76	0.65
1:C:202:GLY:HA2	1:C:291:ARG:HH12	1.61	0.65
1:C:241:LYS:HE2	1:C:314:GLN:O	1.96	0.65
1:F:151:THR:HB	1:F:302:ILE:HG22	1.78	0.65
1:B:34:GLY:HA2	5:B:529:HOH:O	1.96	0.65
1:C:203:GLY:HA3	2:C:401:FLC:OB2	1.95	0.65
1:A:75:VAL:HG13	1:A:118:GLY:CA	2.27	0.65
1:B:99:LEU:HD12	1:B:111:ALA:HA	1.78	0.65
1:D:141:VAL:CG2	1:D:157:MET:HE2	2.26	0.65
1:D:212:PHE:HD1	1:D:327:LEU:HD13	1.62	0.65
1:C:227:ARG:CD	1:C:227:ARG:N	2.38	0.64
1:D:73:CYS:SG	1:D:81:MET:HE2	2.38	0.64
1:C:74:ASP:OD1	1:C:76:GLN:HG2	1.97	0.64
1:C:117:ARG:HH22	1:E:120:GLN:NE2	1.92	0.64
1:F:38:MET:CE	5:F:531:HOH:O	2.44	0.64
1:F:190:TYR:HB2	4:F:402:NAD:C5N	2.26	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:ARG:CD	1:E:227:ARG:N	2.60	0.64
1:A:277:LYS:CE	3:A:402:PE8:H122	2.27	0.64
1:A:75:VAL:HG13	1:A:118:GLY:HA3	1.79	0.64
1:A:118:GLY:O	1:A:122:VAL:HG23	1.98	0.64
1:B:126:ALA:HA	1:B:131:LEU:HB2	1.78	0.64
1:F:308:ARG:NH1	1:F:314:GLN:OE1	2.31	0.64
1:D:117:ARG:HG2	1:D:117:ARG:NH1	2.00	0.64
1:C:113:SER:O	1:C:117:ARG:HG2	1.98	0.63
1:E:234:MET:HE3	1:E:238:ASP:HB3	1.81	0.63
1:C:117:ARG:NH2	1:E:120:GLN:HE22	1.93	0.63
1:A:277:LYS:HZ3	3:A:402:PE8:H122	1.62	0.62
1:E:188:VAL:HG13	1:E:261:ILE:HG12	1.80	0.62
1:E:251:ASN:OD1	1:E:257:ARG:NH2	2.30	0.62
1:A:40:LEU:HD11	1:A:244:MET:HE3	1.80	0.62
1:E:292:GLN:O	1:E:296:GLU:HG3	2.00	0.62
1:E:257:ARG:HG3	1:E:257:ARG:HH11	1.65	0.61
1:F:29:VAL:HG11	1:F:41:VAL:CG2	2.30	0.61
1:A:195:SER:HB3	1:A:236:MET:HB2	1.81	0.61
1:A:308:ARG:HG2	1:A:313:TRP:O	2.00	0.61
1:B:241:LYS:HG2	1:B:313:TRP:HZ3	1.65	0.61
1:C:207:TYR:CD1	1:C:225:LEU:HD12	2.35	0.61
1:D:234:MET:HE2	1:D:238:ASP:HB3	1.82	0.61
1:E:26:ARG:HG2	1:E:88:GLN:O	2.00	0.61
1:C:30:THR:O	1:C:96:MET:HB2	2.01	0.61
1:D:38:MET:CE	1:D:198:ALA:HB2	2.31	0.61
1:D:124:GLU:OE2	1:D:124:GLU:HA	2.00	0.61
1:C:162:MET:O	1:C:166:THR:HG23	2.01	0.61
1:F:314:GLN:OE1	1:F:314:GLN:HA	2.01	0.61
1:B:212:PHE:HD1	1:B:327:LEU:HD13	1.66	0.60
1:C:120:GLN:NE2	1:E:117:ARG:HH22	1.95	0.60
1:C:128:GLN:NE2	5:C:502:HOH:O	2.34	0.60
1:E:242:ALA:CB	1:E:261:ILE:HD13	2.30	0.60
1:D:33:THR:HG21	1:D:59:LYS:HG2	1.82	0.60
1:F:47:LEU:CD1	1:F:244:MET:HE3	2.32	0.60
1:F:99:LEU:HD12	1:F:111:ALA:HA	1.83	0.60
1:F:241:LYS:HG2	1:F:313:TRP:HZ3	1.66	0.60
1:C:117:ARG:NH2	1:E:117:ARG:HH21	1.98	0.60
1:E:40:LEU:O	1:E:44:MET:HG3	2.02	0.60
1:A:119:ILE:HD13	1:A:170:VAL:HG13	1.83	0.60
1:F:75:VAL:CG1	1:F:118:GLY:CA	2.79	0.60
1:D:35:GLN:NE2	2:D:401:FLC:OA1	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:THR:O	1:F:96:MET:HB2	2.02	0.60
1:F:113:SER:O	1:F:117:ARG:HB3	2.02	0.59
1:B:44:MET:CB	1:B:53:ILE:HD11	2.31	0.59
1:C:212:PHE:HD1	1:C:327:LEU:HD13	1.67	0.59
1:F:100:LEU:CD2	4:F:402:NAD:O2A	2.50	0.59
2:E:401:FLC:HA1	4:E:403:NAD:C7N	2.32	0.59
1:E:138:THR:O	1:E:141:VAL:HG22	2.03	0.59
1:C:35:GLN:HE22	4:C:402:NAD:H72N	1.50	0.59
1:D:261:ILE:O	1:D:302:ILE:HD11	2.02	0.59
1:F:257:ARG:HG3	1:F:257:ARG:HH11	1.67	0.59
1:E:199:LEU:H	1:E:199:LEU:HD23	1.66	0.59
1:C:244:MET:HE2	1:C:244:MET:HA	1.84	0.59
1:C:227:ARG:NH1	5:C:501:HOH:O	2.24	0.59
1:B:190:TYR:HD1	1:B:261:ILE:HD11	1.66	0.58
1:C:26:ARG:HD2	1:C:52:THR:HA	1.86	0.58
1:A:260:ASN:HB3	1:A:302:ILE:HD12	1.84	0.58
1:D:56:SER:HA	1:D:71:VAL:O	2.03	0.58
1:D:227:ARG:HD2	1:D:227:ARG:N	2.18	0.58
1:E:33:THR:CG2	1:E:59:LYS:HB2	2.30	0.58
1:E:178:TYR:CD2	1:E:257:ARG:HD3	2.38	0.58
1:A:277:LYS:HB2	3:A:402:PE8:C2	2.30	0.58
1:B:29:VAL:HG11	1:B:41:VAL:HG22	1.84	0.58
1:A:234:MET:CE	1:A:238:ASP:O	2.52	0.57
1:D:99:LEU:HD12	1:D:111:ALA:HA	1.86	0.57
1:A:81:MET:HE2	1:A:125:LEU:CD2	2.33	0.57
1:C:48:PHE:O	1:C:52:THR:HG21	2.05	0.57
1:F:44:MET:HG2	1:F:244:MET:HE1	1.84	0.57
1:B:190:TYR:CD1	1:B:261:ILE:HD11	2.39	0.57
1:C:190:TYR:HB2	4:C:402:NAD:C5N	2.34	0.57
1:A:211:ILE:HG13	1:A:221:TYR:CD2	2.40	0.57
1:A:100:LEU:HD13	2:A:401:FLC:HA2	1.87	0.57
1:A:242:ALA:CB	1:A:261:ILE:HD12	2.35	0.57
1:B:250:PRO:O	1:B:253:CYS:HB2	2.05	0.57
1:D:234:MET:CE	1:D:238:ASP:HB3	2.35	0.57
1:A:212:PHE:HD1	1:A:327:LEU:HD13	1.70	0.56
1:B:35:GLN:NE2	4:B:402:NAD:H72N	1.99	0.56
1:B:29:VAL:HG11	1:B:41:VAL:CG2	2.34	0.56
1:F:75:VAL:HG11	1:F:95:HIS:HE1	1.71	0.56
1:B:268:PRO:O	1:B:272:VAL:HG23	2.05	0.56
1:F:242:ALA:HB2	1:F:313:TRP:CH2	2.40	0.56
1:F:277:LYS:HA	5:F:538:HOH:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:GLN:NE2	4:C:402:NAD:H72N	2.03	0.56
1:F:75:VAL:CG1	1:F:118:GLY:HA3	2.35	0.56
1:B:262:THR:HB	1:B:302:ILE:HG12	1.88	0.56
1:C:234:MET:CE	1:C:238:ASP:HB3	2.35	0.56
1:E:25:SER:O	1:E:26:ARG:HB2	2.06	0.56
2:E:401:FLC:OG1	4:E:403:NAD:C5N	2.54	0.56
1:F:234:MET:HE2	1:F:238:ASP:HB3	1.88	0.55
1:C:172:LEU:HD11	1:E:168:VAL:HG21	1.87	0.55
1:F:66:ARG:HG2	1:F:67:ASP:H	1.71	0.55
1:F:227:ARG:O	1:F:269:GLU:HB2	2.06	0.55
1:C:262:THR:HB	1:C:302:ILE:HG12	1.88	0.55
1:F:74:ASP:OD1	1:F:76:GLN:HG2	2.07	0.55
1:A:242:ALA:HB1	1:A:261:ILE:HD13	1.87	0.55
1:C:29:VAL:HG11	1:C:41:VAL:HG22	1.88	0.54
1:D:75:VAL:HA	1:D:81:MET:CE	2.34	0.54
1:F:45:ARG:NH2	1:F:69:ASN:HB3	2.22	0.54
1:A:234:MET:CE	1:A:238:ASP:C	2.81	0.54
1:C:45:ARG:HB3	1:C:50:ALA:HA	1.90	0.54
1:E:200:PRO:HB3	1:E:209:VAL:CG2	2.37	0.54
1:B:39:GLU:OE2	1:B:236:MET:HE3	2.08	0.54
1:E:289:ASP:OD1	1:E:291:ARG:HG2	2.06	0.54
1:A:178:TYR:CD2	1:A:257:ARG:HD3	2.43	0.54
1:F:52:THR:C	1:F:53:ILE:HD12	2.32	0.54
1:F:251:ASN:OD1	1:F:257:ARG:NH2	2.34	0.54
1:C:157:MET:HE1	1:C:189:ARG:NH2	2.21	0.54
1:E:25:SER:N	2:E:402:FLC:OG2	2.41	0.54
1:F:260:ASN:HB3	1:F:302:ILE:HD12	1.89	0.54
1:A:234:MET:HE2	1:A:238:ASP:C	2.33	0.54
1:A:277:LYS:HE2	3:A:402:PE8:H142	1.90	0.54
1:D:38:MET:HE1	1:D:198:ALA:CB	2.38	0.54
1:A:242:ALA:CB	1:A:261:ILE:CD1	2.87	0.53
1:D:100:LEU:HD11	4:D:403:NAD:H2D	1.90	0.53
1:E:26:ARG:NH1	1:E:88:GLN:O	2.38	0.53
1:E:242:ALA:HB1	1:E:261:ILE:HD13	1.89	0.53
1:C:188:VAL:HG11	1:C:261:ILE:CD1	2.39	0.53
1:A:280:PRO:HB3	3:A:402:PE8:H231	1.90	0.53
1:A:320:ASP:O	1:A:324:GLU:HG3	2.08	0.53
1:C:48:PHE:O	1:C:52:THR:CG2	2.57	0.53
1:E:35:GLN:HG3	1:E:198:ALA:HB3	1.90	0.53
1:E:133:VAL:HG22	1:E:185:PHE:CD2	2.43	0.53
1:F:144:PRO:HD3	1:F:297:THR:HB	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ARG:HG2	1:C:313:TRP:O	2.09	0.53
1:D:78:ARG:HH11	1:D:78:ARG:CG	2.11	0.53
1:B:136:PRO:HB3	1:B:190:TYR:CE2	2.43	0.53
1:B:100:LEU:CD1	2:B:401:FLC:HA2	2.30	0.53
1:C:110:LEU:O	1:C:111:ALA:C	2.48	0.53
1:D:135:ALA:O	1:D:187:SER:CB	2.57	0.53
1:E:308:ARG:HG2	1:E:313:TRP:O	2.08	0.53
1:F:266:PHE:HB2	1:F:270:GLU:HG3	1.91	0.53
1:D:32:GLY:HA3	1:D:55:ASN:OD1	2.08	0.53
1:E:308:ARG:HH12	1:E:315:HIS:HD2	1.57	0.53
1:F:100:LEU:HD23	4:F:402:NAD:O2A	2.09	0.53
1:F:212:PHE:CD2	1:F:326:MET:HE2	2.44	0.53
1:F:32:GLY:HA3	1:F:55:ASN:OD1	2.09	0.52
1:B:137:SER:HB3	1:B:189:ARG:HG2	1.91	0.52
1:D:158:ARG:NH2	1:F:175:GLU:OE1	2.42	0.52
1:F:119:ILE:HG21	1:F:170:VAL:HG22	1.90	0.52
1:F:212:PHE:HD1	1:F:327:LEU:HD13	1.74	0.52
1:C:226:ASN:H	1:C:292:GLN:NE2	2.07	0.52
1:E:118:GLY:O	1:E:122:VAL:HG23	2.08	0.52
1:A:165:LEU:HD12	1:A:165:LEU:C	2.34	0.52
1:E:35:GLN:HA	1:E:198:ALA:HB2	1.90	0.52
1:A:215:ALA:O	1:A:279:MET:HE1	2.09	0.52
1:A:222:THR:HG22	5:A:538:HOH:O	2.10	0.52
1:B:26:ARG:NH1	1:B:88:GLN:O	2.41	0.52
1:B:40:LEU:HD11	1:B:244:MET:HE3	1.91	0.52
1:F:48:PHE:HE2	1:F:244:MET:HE1	1.73	0.52
1:C:228:ASP:N	1:C:228:ASP:OD2	2.43	0.52
1:B:75:VAL:HG13	1:B:118:GLY:CA	2.40	0.52
1:A:235:TYR:HB2	1:A:322:MET:HE2	1.91	0.52
1:B:74:ASP:OD1	1:B:76:GLN:HG2	2.09	0.52
1:C:236:MET:O	1:C:239:CYS:HB3	2.08	0.52
1:C:128:GLN:HB3	5:C:502:HOH:O	2.10	0.51
1:C:75:VAL:HG13	1:C:118:GLY:CA	2.40	0.51
1:A:76:GLN:NE2	1:A:113:SER:OG	2.44	0.51
1:A:234:MET:HE2	1:A:239:CYS:N	2.25	0.51
1:D:78:ARG:HH21	1:D:124:GLU:HG3	1.73	0.51
1:E:133:VAL:HG22	1:E:185:PHE:HD2	1.75	0.51
1:E:267:THR:O	1:E:268:PRO:C	2.53	0.51
1:F:128:GLN:HG3	1:F:129:TYR:CD2	2.46	0.51
1:A:99:LEU:HD12	1:A:111:ALA:HA	1.93	0.51
1:F:276:GLN:HA	1:F:279:MET:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:SER:HB3	1:B:236:MET:HE2	1.93	0.51
1:A:100:LEU:HD11	4:A:403:NAD:O3	2.11	0.51
1:A:302:ILE:CD1	5:A:540:HOH:O	2.58	0.51
2:A:401:FLC:OG1	4:A:403:NAD:C5N	2.58	0.51
1:C:212:PHE:HB3	1:C:330:LEU:HD23	1.93	0.51
1:D:210:GLU:OE1	1:D:224:PHE:HE2	1.93	0.51
1:F:75:VAL:CG1	1:F:118:GLY:HA2	2.40	0.51
1:B:197:GLU:HA	1:B:333:LYS:NZ	2.25	0.50
1:B:75:VAL:HG13	1:B:118:GLY:HA2	1.92	0.50
1:D:33:THR:HG21	1:D:59:LYS:CG	2.39	0.50
1:D:199:LEU:CD2	1:D:199:LEU:H	2.24	0.50
1:A:302:ILE:HD12	5:A:540:HOH:O	2.11	0.50
1:C:99:LEU:HD12	1:C:111:ALA:HA	1.93	0.50
1:C:329:LYS:O	1:C:332:ALA:HB3	2.11	0.50
1:F:68:GLY:O	1:F:69:ASN:HB2	2.09	0.50
1:B:188:VAL:HG22	1:B:261:ILE:HG23	1.93	0.50
1:B:216:LEU:HD23	1:B:330:LEU:HB3	1.94	0.50
1:E:146:THR:O	1:E:148:GLN:HG3	2.12	0.50
1:F:268:PRO:O	1:F:272:VAL:HG23	2.12	0.50
1:C:120:GLN:HE22	1:E:117:ARG:NH2	1.99	0.50
1:A:70:PHE:HE2	1:E:86:THR:CG2	2.25	0.50
1:A:242:ALA:HB1	1:A:261:ILE:CD1	2.42	0.50
1:A:75:VAL:HG13	1:A:118:GLY:HA2	1.93	0.50
1:D:78:ARG:HD2	1:D:125:LEU:CD1	2.41	0.50
1:B:27:ILE:HG23	1:B:92:THR:HB	1.94	0.49
1:C:75:VAL:HG13	1:C:118:GLY:HA2	1.94	0.49
1:C:195:SER:HB2	5:C:533:HOH:O	2.11	0.49
1:E:289:ASP:OD1	1:E:291:ARG:CG	2.59	0.49
1:B:81:MET:HE1	1:B:122:VAL:HG22	1.94	0.49
1:F:100:LEU:HD21	4:F:402:NAD:O2A	2.12	0.49
1:A:34:GLY:O	1:A:38:MET:HB2	2.11	0.49
1:A:277:LYS:HE2	3:A:402:PE8:H122	1.94	0.49
1:B:56:SER:HA	1:B:71:VAL:O	2.13	0.49
1:D:234:MET:HE2	1:D:238:ASP:CB	2.41	0.49
1:F:35:GLN:HG3	1:F:198:ALA:HB3	1.94	0.49
1:B:70:PHE:HE2	1:F:86:THR:HG22	1.76	0.49
1:C:188:VAL:HG23	1:C:246:LEU:HD23	1.93	0.49
1:D:277:LYS:NZ	3:D:402:PE8:C17	2.73	0.49
1:D:309:LYS:HD3	1:D:310:ASP:OD1	2.13	0.49
1:E:226:ASN:H	1:E:292:GLN:HE21	1.57	0.49
1:C:172:LEU:HD12	1:E:168:VAL:HG21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:LEU:HD12	1:F:166:THR:N	2.28	0.49
1:F:128:GLN:HG3	1:F:129:TYR:CE2	2.48	0.49
1:D:73:CYS:SG	1:D:81:MET:CE	3.00	0.48
1:A:137:SER:HB3	1:A:189:ARG:HG2	1.95	0.48
1:C:234:MET:HE2	1:C:238:ASP:HB3	1.94	0.48
1:E:30:THR:OG1	1:E:95:HIS:HA	2.12	0.48
1:E:213:TYR:HB3	5:E:513:HOH:O	2.12	0.48
1:C:234:MET:HE2	1:C:239:CYS:N	2.29	0.48
1:E:29:VAL:HA	1:E:94:VAL:O	2.14	0.48
1:E:212:PHE:HB3	1:E:330:LEU:HD12	1.95	0.48
1:A:26:ARG:HD3	1:A:52:THR:HA	1.94	0.48
1:D:226:ASN:H	1:D:292:GLN:HE21	1.61	0.48
1:B:226:ASN:H	1:B:292:GLN:NE2	2.11	0.48
1:F:156:ILE:HG22	5:F:510:HOH:O	2.14	0.48
1:A:40:LEU:HA	1:A:240:LEU:HD22	1.96	0.48
3:A:402:PE8:H21	3:A:402:PE8:H51	1.63	0.48
1:B:33:THR:HG21	1:B:59:LYS:HG3	1.94	0.48
1:D:137:SER:O	4:D:403:NAD:H6N	2.14	0.48
2:F:401:FLC:HG2	4:F:402:NAD:C7N	2.44	0.48
1:C:110:LEU:HB2	5:C:552:HOH:O	2.13	0.47
1:E:276:GLN:NE2	5:E:502:HOH:O	2.45	0.47
1:F:56:SER:HA	1:F:71:VAL:O	2.13	0.47
1:F:323:VAL:O	1:F:327:LEU:HB2	2.14	0.47
1:B:34:GLY:HA3	4:B:402:NAD:O5B	2.14	0.47
1:E:35:GLN:HA	1:E:198:ALA:CB	2.43	0.47
1:F:100:LEU:HD11	4:F:402:NAD:H2D	1.95	0.47
1:E:191:PRO:HG2	1:E:234:MET:HB3	1.96	0.47
1:E:257:ARG:HG3	1:E:257:ARG:NH1	2.26	0.47
1:A:184:ASP:OD1	1:A:184:ASP:C	2.57	0.47
1:B:129:TYR:HB2	1:B:131:LEU:HD22	1.97	0.47
1:C:136:PRO:HB3	1:C:190:TYR:CE2	2.49	0.47
1:D:41:VAL:HB	1:D:42:PRO:HD3	1.97	0.47
1:D:278:VAL:HG22	3:D:402:PE8:H231	1.96	0.47
1:A:257:ARG:HH11	1:A:257:ARG:CG	2.16	0.47
2:A:401:FLC:HA1	4:A:403:NAD:C7N	2.45	0.47
1:B:44:MET:C	1:B:53:ILE:HD11	2.40	0.47
1:B:45:ARG:HG3	1:B:53:ILE:HD12	1.97	0.47
1:D:257:ARG:HA	1:D:257:ARG:HD3	1.68	0.47
1:B:165:LEU:C	1:B:165:LEU:HD12	2.39	0.47
1:C:99:LEU:CD1	1:C:114:VAL:HG21	2.44	0.47
1:E:272:VAL:O	1:E:276:GLN:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:VAL:HG13	1:C:55:ASN:HA	1.96	0.47
1:C:293:GLN:O	1:C:297:THR:HG23	2.16	0.47
1:C:212:PHE:CD1	1:C:327:LEU:HD13	2.47	0.46
1:E:194:ILE:HG23	1:E:326:MET:HE2	1.96	0.46
1:F:171:GLU:OE1	1:F:189:ARG:NH2	2.49	0.46
1:C:226:ASN:H	1:C:292:GLN:HE21	1.63	0.46
1:D:38:MET:HE1	1:D:198:ALA:N	2.29	0.46
1:E:234:MET:HE3	1:E:238:ASP:C	2.40	0.46
2:F:401:FLC:CG	4:F:402:NAD:C7N	2.93	0.46
1:A:213:TYR:CZ	1:A:330:LEU:HD21	2.50	0.46
1:D:100:LEU:HD13	1:D:163:TYR:CE1	2.50	0.46
1:D:190:TYR:HB2	4:D:403:NAD:C5N	2.45	0.46
1:D:277:LYS:HG3	3:D:402:PE8:H241	1.97	0.46
1:E:243:THR:O	1:E:247:ILE:HG13	2.16	0.46
1:F:35:GLN:NE2	4:F:402:NAD:H72N	2.14	0.46
1:F:66:ARG:HG2	1:F:67:ASP:N	2.31	0.46
1:C:212:PHE:HZ	1:C:323:VAL:HG22	1.81	0.46
1:C:224:PHE:O	1:C:288:PRO:HA	2.16	0.46
1:E:251:ASN:ND2	1:E:251:ASN:O	2.49	0.46
1:B:264:VAL:HG11	1:B:318:ASP:HA	1.97	0.45
1:F:241:LYS:HG2	1:F:313:TRP:CZ3	2.50	0.45
1:D:45:ARG:HH12	1:D:67:ASP:CG	2.25	0.45
1:E:157:MET:HE1	1:E:189:ARG:NH2	2.32	0.45
1:E:251:ASN:HD21	1:E:257:ARG:HH21	1.64	0.45
3:A:402:PE8:H142	3:A:402:PE8:H172	1.68	0.45
1:F:257:ARG:HG3	1:F:257:ARG:NH1	2.32	0.45
1:B:99:LEU:HD11	1:B:110:LEU:HG	1.98	0.45
1:E:85:VAL:HA	1:E:90:VAL:CG2	2.46	0.45
1:E:92:THR:HA	1:E:132:ARG:O	2.17	0.45
1:D:92:THR:HG23	1:D:132:ARG:HG3	1.97	0.45
1:A:333:LYS:HE2	1:A:333:LYS:HB3	1.85	0.45
1:B:43:TYR:O	1:B:46:GLN:HB2	2.15	0.45
1:A:30:THR:O	1:A:96:MET:HB2	2.17	0.45
1:B:70:PHE:HE2	1:F:86:THR:CG2	2.30	0.45
1:B:185:PHE:CD1	1:B:185:PHE:C	2.94	0.45
1:C:110:LEU:HA	5:C:552:HOH:O	2.16	0.45
1:C:330:LEU:O	1:C:334:LEU:HD12	2.17	0.45
1:D:66:ARG:HA	1:D:66:ARG:HD2	1.81	0.45
1:D:266:PHE:CD2	1:D:319:LEU:HD13	2.52	0.45
1:E:251:ASN:CG	1:E:257:ARG:HH22	2.22	0.45
1:D:199:LEU:H	1:D:199:LEU:HD22	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:LEU:HG	2:F:401:FLC:HA2	1.98	0.45
1:B:188:VAL:HG22	1:B:261:ILE:CG2	2.46	0.45
1:B:232:PRO:HD3	1:B:299:PRO:O	2.17	0.45
1:A:234:MET:HE3	1:A:238:ASP:HB3	1.99	0.44
1:C:78:ARG:O	1:C:81:MET:HB3	2.16	0.44
1:D:34:GLY:HA3	4:D:403:NAD:O5B	2.18	0.44
1:A:229:ALA:O	1:A:268:PRO:HD3	2.17	0.44
1:C:188:VAL:HG23	1:C:246:LEU:CD2	2.46	0.44
1:D:173:LEU:HD11	1:F:162:MET:HE1	1.99	0.44
1:E:308:ARG:HH12	1:E:315:HIS:CD2	2.34	0.44
1:A:234:MET:HE2	1:A:238:ASP:O	2.16	0.44
1:D:199:LEU:HD22	1:D:199:LEU:N	2.33	0.44
1:D:267:THR:O	1:D:268:PRO:C	2.57	0.44
1:B:195:SER:O	1:B:326:MET:HE1	2.16	0.44
1:C:99:LEU:CG	1:C:114:VAL:HG21	2.42	0.44
1:E:174:GLY:HA3	1:E:185:PHE:CE1	2.53	0.44
1:A:81:MET:HE2	1:A:125:LEU:HD23	1.99	0.44
1:A:320:ASP:OD1	3:A:402:PE8:H81	2.18	0.44
1:D:44:MET:HE3	1:D:244:MET:HE1	1.99	0.44
1:B:48:PHE:O	1:B:52:THR:HG21	2.18	0.44
1:D:185:PHE:CD1	1:D:185:PHE:C	2.96	0.44
1:A:252:ASP:OD2	1:A:252:ASP:N	2.47	0.44
1:B:200:PRO:HB3	1:B:209:VAL:CG2	2.46	0.44
1:B:108:PRO:HB2	5:B:544:HOH:O	2.17	0.44
1:C:133:VAL:HG22	1:C:185:PHE:CD2	2.52	0.44
1:C:78:ARG:HD2	1:C:125:LEU:HD13	2.00	0.43
1:A:220:LYS:HA	1:A:283:GLN:O	2.18	0.43
1:B:45:ARG:O	1:B:49:GLY:N	2.50	0.43
1:B:211:ILE:HG13	1:B:221:TYR:CD2	2.53	0.43
1:E:74:ASP:HA	4:E:403:NAD:N1A	2.33	0.43
1:E:318:ASP:OD1	1:E:321:SER:OG	2.35	0.43
1:F:151:THR:HA	1:F:152:PRO:HD3	1.74	0.43
1:B:30:THR:O	1:B:96:MET:HB2	2.18	0.43
1:F:230:LYS:H	1:F:300:ARG:HH12	1.67	0.43
1:E:211:ILE:HG13	1:E:221:TYR:CD2	2.53	0.43
1:F:47:LEU:HD12	1:F:244:MET:HE3	2.01	0.43
1:C:35:GLN:NE2	4:C:402:NAD:N7N	2.66	0.43
1:B:223:CYS:HB3	1:B:286:TYR:CD2	2.54	0.43
1:E:81:MET:HE1	1:E:122:VAL:HG22	2.01	0.43
1:F:212:PHE:CD1	1:F:327:LEU:HD13	2.53	0.43
1:F:250:PRO:O	1:F:251:ASN:C	2.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LYS:HE2	5:C:557:HOH:O	2.18	0.43
1:C:172:LEU:HD12	1:E:168:VAL:CG2	2.47	0.43
1:E:141:VAL:HB	1:E:168:VAL:HG12	2.00	0.43
1:E:212:PHE:HD1	1:E:327:LEU:HD13	1.83	0.43
1:E:223:CYS:HB3	1:E:286:TYR:CD2	2.53	0.43
1:F:332:ALA:C	1:F:334:LEU:H	2.27	0.43
1:C:290:PHE:O	1:C:293:GLN:HG2	2.19	0.43
1:D:81:MET:HE3	1:D:81:MET:HB2	1.82	0.43
1:A:78:ARG:HH21	1:A:124:GLU:HG2	1.84	0.43
1:B:278:VAL:HG21	1:B:324:GLU:HG2	2.01	0.43
1:F:165:LEU:HD12	1:F:165:LEU:C	2.44	0.43
1:E:99:LEU:CD1	1:E:110:LEU:HG	2.49	0.42
1:E:280:PRO:HD2	5:E:537:HOH:O	2.18	0.42
1:B:330:LEU:HD12	1:B:330:LEU:HA	1.59	0.42
1:E:195:SER:HB3	1:E:236:MET:HB2	2.01	0.42
1:A:40:LEU:HD11	1:A:244:MET:CE	2.46	0.42
1:A:212:PHE:CD1	1:A:327:LEU:HD13	2.53	0.42
1:A:215:ALA:O	1:A:219:GLY:HA2	2.19	0.42
1:D:48:PHE:O	1:D:52:THR:HG21	2.19	0.42
1:C:230:LYS:C	1:C:231:LEU:HG	2.44	0.42
1:C:142:PHE:HB2	1:C:299:PRO:HD3	2.01	0.42
1:B:197:GLU:HA	1:B:197:GLU:OE1	2.19	0.42
1:D:234:MET:HE1	1:D:313:TRP:CZ2	2.55	0.42
1:A:78:ARG:NH1	1:A:78:ARG:HG2	2.34	0.42
1:A:277:LYS:HZ1	3:A:402:PE8:H122	1.79	0.42
1:B:227:ARG:HH11	1:B:227:ARG:H	1.68	0.42
1:F:33:THR:O	1:F:33:THR:HG22	2.20	0.42
1:B:203:GLY:O	1:B:206:ASP:HB2	2.19	0.42
1:D:117:ARG:HH11	1:D:117:ARG:CG	2.09	0.42
1:F:234:MET:CE	1:F:313:TRP:CZ2	3.02	0.42
1:A:292:GLN:OE1	1:A:296:GLU:HG2	2.20	0.41
1:E:35:GLN:NE2	4:E:403:NAD:H72N	2.17	0.41
1:A:30:THR:OG1	1:A:95:HIS:HA	2.19	0.41
1:A:232:PRO:C	1:A:233:MET:HG2	2.45	0.41
1:B:79:ASP:O	1:B:82:ALA:HB3	2.20	0.41
1:D:38:MET:HE2	1:D:38:MET:HB3	1.72	0.41
1:D:266:PHE:CE2	1:D:319:LEU:HD13	2.55	0.41
1:F:44:MET:CG	1:F:244:MET:HE2	2.44	0.41
1:F:48:PHE:O	1:F:52:THR:HG21	2.21	0.41
1:A:138:THR:O	1:A:141:VAL:HG22	2.21	0.41
1:C:123:LEU:HD11	1:C:174:GLY:HA2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:CD1	1:E:168:VAL:CG2	2.96	0.41
1:E:120:GLN:O	1:E:124:GLU:HB2	2.20	0.41
1:E:264:VAL:HG11	1:E:318:ASP:HA	2.01	0.41
1:A:226:ASN:H	1:A:292:GLN:NE2	2.18	0.41
1:D:38:MET:HE1	1:D:198:ALA:CA	2.51	0.41
1:F:259:TYR:HE1	1:F:306:ILE:HG22	1.85	0.41
1:C:212:PHE:CZ	1:C:323:VAL:HG22	2.56	0.41
1:D:34:GLY:O	1:D:38:MET:HB2	2.21	0.41
1:D:124:GLU:CD	1:D:127:LYS:HE3	2.44	0.41
1:C:29:VAL:CG1	1:C:55:ASN:HA	2.51	0.41
1:C:135:ALA:HA	1:C:136:PRO:HD2	1.77	0.41
1:D:332:ALA:O	1:D:334:LEU:N	2.52	0.41
1:F:242:ALA:HB2	1:F:313:TRP:CZ3	2.54	0.41
1:C:81:MET:CE	1:C:122:VAL:HG22	2.31	0.41
1:D:225:LEU:O	1:D:226:ASN:C	2.63	0.41
1:B:257:ARG:HG3	1:B:257:ARG:NH1	2.24	0.41
1:C:77:ASP:OD1	1:C:77:ASP:C	2.64	0.41
1:C:110:LEU:O	1:C:114:VAL:HG22	2.20	0.41
1:C:113:SER:O	1:C:114:VAL:C	2.62	0.41
1:D:277:LYS:HZ3	3:D:402:PE8:C17	2.33	0.41
2:B:401:FLC:HA1	4:B:402:NAD:N7N	2.36	0.41
1:C:188:VAL:CG1	1:C:261:ILE:HD13	2.45	0.41
1:C:235:TYR:CG	1:C:237:PRO:HD2	2.56	0.41
1:C:242:ALA:CB	1:C:261:ILE:HD12	2.50	0.41
1:E:234:MET:CE	1:E:238:ASP:C	2.94	0.41
1:E:308:ARG:HH22	1:E:315:HIS:CD2	2.38	0.41
1:A:234:MET:HE3	1:A:238:ASP:C	2.45	0.41
1:B:151:THR:HA	1:B:152:PRO:HD3	1.92	0.41
1:C:169:HIS:O	1:C:170:VAL:C	2.64	0.41
1:C:195:SER:CB	5:C:533:HOH:O	2.69	0.41
1:F:268:PRO:O	1:F:269:GLU:C	2.62	0.41
1:A:48:PHE:O	1:A:52:THR:HG21	2.20	0.40
1:A:75:VAL:CG1	1:A:118:GLY:HA3	2.48	0.40
1:F:267:THR:H	1:F:270:GLU:HG2	1.86	0.40
1:A:83:ARG:O	1:A:87:GLU:HB2	2.21	0.40
1:B:33:THR:HG21	1:B:59:LYS:CG	2.50	0.40
1:F:305:SER:HA	1:F:308:ARG:HG3	2.02	0.40
1:A:185:PHE:O	1:A:257:ARG:NH1	2.53	0.40
1:F:132:ARG:NH2	1:F:247:ILE:O	2.39	0.40
1:B:112:LEU:O	1:B:116:THR:HG23	2.22	0.40
1:D:329:LYS:O	1:D:332:ALA:HB3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:PRO:HG2	4:B:402:NAD:H4D	2.03	0.40
1:C:134:PHE:CE2	1:C:136:PRO:HD3	2.56	0.40
1:C:202:GLY:HA2	1:C:291:ARG:NH1	2.32	0.40
1:C:326:MET:O	1:C:330:LEU:HB2	2.22	0.40
1:D:27:ILE:HB	1:D:53:ILE:HD12	2.03	0.40
1:D:320:ASP:HB3	3:D:402:PE8:H242	2.04	0.40
1:E:25:SER:O	1:E:26:ARG:CB	2.68	0.40
1:E:34:GLY:O	1:E:38:MET:HG2	2.22	0.40
1:E:100:LEU:HD11	4:E:403:NAD:H2D	2.03	0.40
1:F:174:GLY:HA3	1:F:185:PHE:CE1	2.57	0.40
1:F:203:GLY:O	1:F:206:ASP:HB2	2.21	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	302/345 (88%)	280 (93%)	22 (7%)	0	100	100
1	B	302/345 (88%)	287 (95%)	15 (5%)	0	100	100
1	C	302/345 (88%)	282 (93%)	20 (7%)	0	100	100
1	D	303/345 (88%)	288 (95%)	11 (4%)	4 (1%)	9	10
1	E	300/345 (87%)	284 (95%)	14 (5%)	2 (1%)	18	22
1	F	303/345 (88%)	281 (93%)	20 (7%)	2 (1%)	18	22
All	All	1812/2070 (88%)	1702 (94%)	102 (6%)	8 (0%)	30	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	67	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	227	ARG
1	E	26	ARG
1	F	69	ASN
1	D	184	ASP
1	F	333	LYS
1	D	333	LYS
1	E	227	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	265/293 (90%)	241 (91%)	24 (9%)	9	11
1	B	265/293 (90%)	236 (89%)	29 (11%)	6	7
1	C	265/293 (90%)	232 (88%)	33 (12%)	4	4
1	D	266/293 (91%)	238 (90%)	28 (10%)	6	7
1	E	263/293 (90%)	235 (89%)	28 (11%)	6	7
1	F	266/293 (91%)	242 (91%)	24 (9%)	9	11
All	All	1590/1758 (90%)	1424 (90%)	166 (10%)	7	8

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	29	VAL
1	A	33	THR
1	A	47	LEU
1	A	52	THR
1	A	75	VAL
1	A	78	ARG
1	A	79	ASP
1	A	117	ARG
1	A	125	LEU
1	A	131	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	133	VAL
1	A	138	THR
1	A	150	GLU
1	A	175	GLU
1	A	188	VAL
1	A	216	LEU
1	A	227	ARG
1	A	234	MET
1	A	257	ARG
1	A	302	ILE
1	A	309	LYS
1	A	322	MET
1	A	327	LEU
1	B	33	THR
1	B	38	MET
1	B	52	THR
1	B	59	LYS
1	B	67	ASP
1	B	75	VAL
1	B	76	GLN
1	B	78	ARG
1	B	86	THR
1	B	114	VAL
1	B	117	ARG
1	B	125	LEU
1	B	131	LEU
1	B	133	VAL
1	B	150	GLU
1	B	175	GLU
1	B	188	VAL
1	B	196	SER
1	B	199	LEU
1	B	216	LEU
1	B	227	ARG
1	B	253	CYS
1	B	257	ARG
1	B	277	LYS
1	B	287	LYS
1	B	300	ARG
1	B	305	SER
1	B	327	LEU
1	B	330	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	33	THR
1	C	52	THR
1	C	75	VAL
1	C	78	ARG
1	C	85	VAL
1	C	113	SER
1	C	117	ARG
1	C	125	LEU
1	C	132	ARG
1	C	133	VAL
1	C	150	GLU
1	C	175	GLU
1	C	187	SER
1	C	188	VAL
1	C	209	VAL
1	C	216	LEU
1	C	222	THR
1	C	227	ARG
1	C	234	MET
1	C	246	LEU
1	C	252	ASP
1	C	265	SER
1	C	281	SER
1	C	290	PHE
1	C	293	GLN
1	C	296	GLU
1	C	302	ILE
1	C	309	LYS
1	C	318	ASP
1	C	324	GLU
1	C	327	LEU
1	C	330	LEU
1	C	334	LEU
1	D	29	VAL
1	D	33	THR
1	D	46	GLN
1	D	51	ASP
1	D	52	THR
1	D	59	LYS
1	D	78	ARG
1	D	100	LEU
1	D	117	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	125	LEU
1	D	127	LYS
1	D	133	VAL
1	D	148	GLN
1	D	154	THR
1	D	175	GLU
1	D	188	VAL
1	D	199	LEU
1	D	216	LEU
1	D	220	LYS
1	D	227	ARG
1	D	278	VAL
1	D	293	GLN
1	D	309	LYS
1	D	314	GLN
1	D	323	VAL
1	D	327	LEU
1	D	330	LEU
1	D	334	LEU
1	E	26	ARG
1	E	29	VAL
1	E	33	THR
1	E	35	GLN
1	E	75	VAL
1	E	78	ARG
1	E	86	THR
1	E	100	LEU
1	E	117	ARG
1	E	125	LEU
1	E	127	LYS
1	E	132	ARG
1	E	133	VAL
1	E	158	ARG
1	E	175	GLU
1	E	188	VAL
1	E	199	LEU
1	E	207	TYR
1	E	216	LEU
1	E	227	ARG
1	E	230	LYS
1	E	234	MET
1	E	256	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	257	ARG
1	E	269	GLU
1	E	291	ARG
1	E	321	SER
1	E	327	LEU
1	F	25	SER
1	F	52	THR
1	F	59	LYS
1	F	100	LEU
1	F	117	ARG
1	F	119	ILE
1	F	125	LEU
1	F	130	GLN
1	F	133	VAL
1	F	150	GLU
1	F	154	THR
1	F	188	VAL
1	F	206	ASP
1	F	216	LEU
1	F	227	ARG
1	F	241	LYS
1	F	257	ARG
1	F	261	ILE
1	F	277	LYS
1	F	300	ARG
1	F	309	LYS
1	F	321	SER
1	F	327	LEU
1	F	328	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	76	GLN
1	A	88	GLN
1	A	120	GLN
1	A	121	ASN
1	A	314	GLN
1	A	315	HIS
1	B	35	GLN
1	B	46	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	55	ASN
1	B	69	ASN
1	B	76	GLN
1	B	120	GLN
1	B	121	ASN
1	B	256	GLN
1	B	283	GLN
1	B	292	GLN
1	B	315	HIS
1	C	35	GLN
1	C	76	GLN
1	C	120	GLN
1	C	121	ASN
1	C	256	GLN
1	C	283	GLN
1	C	292	GLN
1	C	312	ASN
1	C	315	HIS
1	D	35	GLN
1	D	76	GLN
1	D	121	ASN
1	D	218	HIS
1	D	256	GLN
1	D	292	GLN
1	D	314	GLN
1	D	315	HIS
1	E	120	GLN
1	E	121	ASN
1	E	148	GLN
1	E	276	GLN
1	E	283	GLN
1	E	292	GLN
1	E	314	GLN
1	E	315	HIS
1	F	35	GLN
1	F	121	ASN
1	F	283	GLN
1	F	292	GLN
1	F	315	HIS

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 ⓘ

15 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	$\# Z > 2$
2	FLC	B	401	-	12,12,12	1.01	0	17,17,17	1.58	4 (23%)
2	FLC	A	401	-	12,12,12	1.46	1 (8%)	17,17,17	1.64	4 (23%)
4	NAD	E	403	-	46,48,48	1.72	7 (15%)	64,73,73	1.89	16 (25%)
4	NAD	A	403	-	46,48,48	1.69	8 (17%)	64,73,73	1.82	12 (18%)
2	FLC	E	402	-	12,12,12	1.77	1 (8%)	17,17,17	2.75	6 (35%)
3	PE8	D	402	-	24,24,24	0.76	0	23,23,23	0.77	0
4	NAD	C	402	-	46,48,48	1.27	5 (10%)	64,73,73	1.61	9 (14%)
3	PE8	A	402	-	24,24,24	0.79	0	23,23,23	0.85	0
4	NAD	B	402	-	46,48,48	1.89	12 (26%)	64,73,73	1.76	20 (31%)
2	FLC	F	401	-	12,12,12	1.44	1 (8%)	17,17,17	1.90	5 (29%)
4	NAD	F	402	-	46,48,48	1.61	8 (17%)	64,73,73	1.98	14 (21%)
2	FLC	E	401	-	12,12,12	1.08	0	17,17,17	1.70	4 (23%)
2	FLC	C	401	-	12,12,12	1.27	1 (8%)	17,17,17	1.19	2 (11%)
4	NAD	D	403	-	46,48,48	1.49	7 (15%)	64,73,73	1.81	13 (20%)
2	FLC	D	401	-	12,12,12	1.39	1 (8%)	17,17,17	1.66	3 (17%)

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
2	FLC	B	401	-	-	6/16/16/16	-
2	FLC	A	401	-	-	13/16/16/16	-
4	NAD	E	403	-	-	3/30/62/62	0/5/5/5
4	NAD	A	403	-	-	5/30/62/62	0/5/5/5
2	FLC	E	402	-	-	5/16/16/16	-
3	PE8	D	402	-	-	13/22/22/22	-
4	NAD	C	402	-	-	4/30/62/62	0/5/5/5
3	PE8	A	402	-	-	14/22/22/22	-
4	NAD	B	402	-	-	1/30/62/62	0/5/5/5
2	FLC	F	401	-	-	6/16/16/16	-
4	NAD	F	402	-	-	2/30/62/62	0/5/5/5
2	FLC	E	401	-	-	8/16/16/16	-
2	FLC	C	401	-	-	6/16/16/16	-
4	NAD	D	403	-	-	2/30/62/62	0/5/5/5
2	FLC	D	401	-	-	9/16/16/16	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	NAD	C5A-C4A	6.75	1.51	1.39
4	A	403	NAD	C5A-C4A	6.30	1.50	1.39
4	D	403	NAD	C5A-C4A	5.52	1.48	1.39
4	F	402	NAD	C5A-C4A	5.28	1.48	1.39
4	F	402	NAD	PN-O3	4.91	1.64	1.59
4	E	403	NAD	C5A-C4A	4.88	1.47	1.39
4	E	403	NAD	O4D-C1D	4.64	1.47	1.40
4	C	402	NAD	C5A-C4A	4.38	1.46	1.39
2	E	402	FLC	CB-CBC	4.33	1.58	1.53
4	E	403	NAD	PN-O3	4.03	1.63	1.59
4	A	403	NAD	C5A-C6A	3.81	1.51	1.41
4	B	402	NAD	PN-O3	3.58	1.63	1.59
4	E	403	NAD	C5A-C6A	3.57	1.50	1.41
4	B	402	NAD	C2N-C3N	3.57	1.44	1.39
4	B	402	NAD	C2N-N1N	3.54	1.38	1.35
4	E	403	NAD	C2N-N1N	3.54	1.38	1.35
4	A	403	NAD	O4D-C1D	3.52	1.45	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	NAD	C2N-N1N	3.48	1.38	1.35
4	D	403	NAD	PN-O3	3.44	1.63	1.59
4	B	402	NAD	C2A-N1A	3.37	1.39	1.33
4	F	402	NAD	PA-O3	3.35	1.63	1.59
4	E	403	NAD	PA-O3	3.27	1.63	1.59
4	E	403	NAD	C2N-C3N	3.23	1.44	1.39
4	B	402	NAD	C5A-C6A	3.14	1.49	1.41
4	D	403	NAD	O4D-C1D	3.10	1.45	1.40
2	A	401	FLC	CB-CBC	-3.06	1.50	1.53
4	C	402	NAD	C8A-N7A	2.96	1.37	1.31
4	A	403	NAD	C8A-N7A	2.91	1.37	1.31
4	D	403	NAD	C5A-C6A	2.85	1.48	1.41
2	C	401	FLC	CB-CBC	-2.81	1.50	1.53
4	D	403	NAD	C8A-N7A	2.80	1.37	1.31
4	B	402	NAD	PA-O3	2.80	1.62	1.59
4	B	402	NAD	C8A-N7A	2.79	1.37	1.31
4	C	402	NAD	O4D-C1D	2.78	1.44	1.40
4	F	402	NAD	O4D-C1D	2.77	1.44	1.40
2	F	401	FLC	CB-CBC	-2.72	1.50	1.53
4	F	402	NAD	C4A-N3A	2.69	1.39	1.34
4	F	402	NAD	C5A-C6A	2.67	1.48	1.41
4	B	402	NAD	C2A-N3A	2.57	1.38	1.33
4	F	402	NAD	C8A-N7A	2.54	1.36	1.31
4	B	402	NAD	C3N-C7N	2.54	1.54	1.50
4	F	402	NAD	C2A-N1A	2.47	1.38	1.33
4	C	402	NAD	C5A-N7A	-2.46	1.34	1.39
2	D	401	FLC	CA-CB	2.33	1.56	1.54
4	C	402	NAD	PN-O3	2.30	1.62	1.59
4	A	403	NAD	C5N-C4N	2.23	1.42	1.38
4	D	403	NAD	PA-O3	2.18	1.61	1.59
4	B	402	NAD	O4D-C1D	2.17	1.43	1.40
4	B	402	NAD	C4A-N9A	-2.16	1.33	1.37
4	D	403	NAD	C4A-N3A	2.04	1.38	1.34
4	A	403	NAD	PN-O3	2.03	1.61	1.59
4	A	403	NAD	C2A-N3A	2.02	1.37	1.33

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	402	FLC	OHB-CB-CBC	6.22	117.78	108.96
4	A	403	NAD	C5A-C4A-N3A	-5.77	118.78	126.72
4	F	402	NAD	C5A-N7A-C8A	5.61	112.26	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	402	NAD	C5A-C4A-N3A	-5.29	119.44	126.72
2	E	402	FLC	OB2-CBC-CB	5.21	123.13	113.14
4	F	402	NAD	C4A-C5A-N7A	-5.19	104.65	110.58
4	E	403	NAD	C5A-C4A-N3A	-5.08	119.72	126.72
4	E	403	NAD	N3A-C4A-N9A	4.94	135.56	127.17
4	F	402	NAD	N9A-C8A-N7A	-4.89	107.00	113.94
4	F	402	NAD	C4A-N9A-C8A	4.83	110.81	105.74
2	F	401	FLC	CB-CG-CGC	4.65	126.63	113.92
4	D	403	NAD	N3A-C2A-N1A	-4.60	121.61	128.58
4	D	403	NAD	C5A-C4A-N3A	-4.57	120.42	126.72
4	C	402	NAD	N3A-C2A-N1A	-4.55	121.70	128.58
4	A	403	NAD	N3A-C4A-N9A	4.47	134.77	127.17
4	E	403	NAD	C4A-N9A-C8A	4.46	110.42	105.74
4	E	403	NAD	N3A-C2A-N1A	-4.46	121.84	128.58
4	A	403	NAD	C2A-N3A-C4A	4.44	122.68	111.83
4	C	402	NAD	N3A-C4A-N9A	4.43	134.71	127.17
4	F	402	NAD	C5A-C4A-N3A	-4.43	120.61	126.72
4	B	402	NAD	C6N-N1N-C1D	-4.40	111.08	119.73
4	A	403	NAD	N3A-C2A-N1A	-4.28	122.10	128.58
4	C	402	NAD	C2A-N3A-C4A	4.28	122.27	111.83
4	E	403	NAD	C2A-N3A-C4A	4.16	122.00	111.83
4	A	403	NAD	C4A-C5A-N7A	-4.15	105.84	110.58
4	D	403	NAD	N3A-C4A-N9A	4.14	134.21	127.17
4	F	402	NAD	N3A-C4A-N9A	4.08	134.11	127.17
2	D	401	FLC	OB2-CBC-CB	3.98	120.78	113.14
4	D	403	NAD	C2A-N3A-C4A	3.83	121.18	111.83
4	D	403	NAD	C4A-N9A-C8A	3.78	109.71	105.74
4	F	402	NAD	N3A-C2A-N1A	-3.77	122.88	128.58
2	A	401	FLC	OHB-CB-CG	3.71	117.83	109.38
2	E	402	FLC	OHB-CB-CA	-3.70	100.94	109.38
4	B	402	NAD	C2N-N1N-C1D	3.69	127.28	119.13
4	B	402	NAD	C5A-C4A-N3A	-3.62	121.73	126.72
4	F	402	NAD	C2A-N1A-C6A	3.59	124.62	118.73
2	E	401	FLC	CB-CA-CAC	3.58	123.71	113.92
2	E	402	FLC	CG-CB-CA	3.57	118.47	109.31
2	E	402	FLC	OHB-CB-CG	-3.56	101.25	109.38
4	A	403	NAD	O4B-C1B-N9A	3.51	114.83	108.09
4	B	402	NAD	N3A-C2A-N1A	-3.45	123.36	128.58
4	B	402	NAD	C4A-N9A-C8A	3.43	109.34	105.74
2	B	401	FLC	OB2-CBC-CB	3.35	119.57	113.14
4	E	403	NAD	N9A-C8A-N7A	-3.32	109.22	113.94
4	B	402	NAD	N3A-C4A-N9A	3.25	132.69	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	402	NAD	C6N-N1N-C1D	-3.19	113.47	119.73
4	E	403	NAD	C5A-N7A-C8A	3.14	108.39	103.45
4	A	403	NAD	C6A-C5A-N7A	3.12	138.11	132.09
4	D	403	NAD	C6A-C5A-N7A	3.12	138.10	132.09
4	D	403	NAD	O4B-C1B-N9A	3.09	114.03	108.09
4	A	403	NAD	C5A-N7A-C8A	3.08	108.28	103.45
2	F	401	FLC	CG-CB-CBC	-3.07	103.25	110.03
4	D	403	NAD	C4A-C5A-N7A	-3.06	107.08	110.58
4	B	402	NAD	C4A-C5A-N7A	-3.03	107.12	110.58
4	F	402	NAD	C6A-C5A-N7A	2.96	137.79	132.09
2	F	401	FLC	OHB-CB-CA	-2.93	102.70	109.38
4	E	403	NAD	C4A-C5A-N7A	-2.91	107.26	110.58
2	C	401	FLC	OG1-CGC-CG	-2.91	114.72	122.95
4	F	402	NAD	C2A-N3A-C4A	2.84	118.77	111.83
4	D	403	NAD	C5A-N7A-C8A	2.80	107.85	103.45
4	B	402	NAD	C2A-N3A-C4A	2.78	118.63	111.83
4	D	403	NAD	N9A-C8A-N7A	-2.78	110.00	113.94
4	F	402	NAD	C4A-N9A-C1B	-2.75	120.20	126.63
4	D	403	NAD	C2A-N1A-C6A	2.73	123.22	118.73
4	E	403	NAD	C2D-C3D-C4D	2.66	107.76	102.61
4	E	403	NAD	C6N-N1N-C1D	-2.66	114.50	119.73
4	E	403	NAD	C2N-N1N-C1D	2.65	124.98	119.13
2	A	401	FLC	OB2-CBC-CB	2.65	118.22	113.14
2	E	401	FLC	CA-CB-CBC	2.63	115.86	110.03
2	E	401	FLC	CG-CB-CA	-2.61	102.61	109.31
4	B	402	NAD	C4A-N9A-C1B	-2.61	120.53	126.63
4	E	403	NAD	C6A-C5A-N7A	2.61	137.12	132.09
2	E	402	FLC	OB2-CBC-OB1	-2.59	115.57	123.86
4	D	403	NAD	C4A-N9A-C1B	-2.56	120.65	126.63
2	D	401	FLC	OHB-CB-CBC	-2.55	105.34	108.96
4	A	403	NAD	C4A-N9A-C8A	2.55	108.41	105.74
4	C	402	NAD	C6A-C5A-N7A	2.54	137.00	132.09
4	B	402	NAD	O3B-C3B-C4B	-2.54	103.79	111.08
4	C	402	NAD	C4A-N9A-C8A	2.50	108.36	105.74
2	B	401	FLC	OHB-CB-CA	-2.49	103.70	109.38
4	B	402	NAD	C2N-C3N-C7N	2.47	126.60	119.46
4	B	402	NAD	C4N-C3N-C7N	-2.43	114.43	121.06
4	B	402	NAD	C6A-C5A-N7A	2.43	136.77	132.09
2	E	401	FLC	OHB-CB-CBC	2.42	112.39	108.96
4	B	402	NAD	O2N-PN-O1N	2.40	123.62	112.44
2	B	401	FLC	OA2-CAC-CA	2.40	121.96	114.35
4	F	402	NAD	O5B-PA-O1A	-2.39	99.46	108.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	403	NAD	C2A-N1A-C6A	2.35	122.60	118.73
2	B	401	FLC	OA1-CAC-CA	-2.29	116.47	122.95
4	E	403	NAD	O7N-C7N-C3N	2.27	122.38	119.60
4	F	402	NAD	C2N-N1N-C1D	2.22	124.03	119.13
4	C	402	NAD	O2A-PA-O1A	2.20	122.68	112.44
4	B	402	NAD	C5A-N7A-C8A	2.20	106.91	103.45
4	C	402	NAD	C5A-C6A-N6A	-2.17	117.90	123.29
4	C	402	NAD	C4A-C5A-N7A	-2.17	108.11	110.58
4	A	403	NAD	O2N-PN-O1N	2.15	122.47	112.44
4	B	402	NAD	C2A-N1A-C6A	2.15	122.27	118.73
2	F	401	FLC	OHB-CB-CBC	2.15	112.01	108.96
2	D	401	FLC	OA2-CAC-OA1	-2.13	117.86	123.33
4	E	403	NAD	O2A-PA-O1A	2.12	122.31	112.44
4	B	402	NAD	O7N-C7N-C3N	2.11	122.18	119.60
4	E	403	NAD	O2N-PN-O1N	2.10	122.22	112.44
2	C	401	FLC	CB-CA-CAC	2.09	119.64	113.92
2	A	401	FLC	CG-CB-CA	-2.09	103.95	109.31
2	A	401	FLC	OHB-CB-CBC	-2.08	106.02	108.96
4	A	403	NAD	N9A-C8A-N7A	-2.06	111.01	113.94
2	F	401	FLC	OB1-CBC-CB	-2.06	118.11	122.09
4	B	402	NAD	O7N-C7N-N7N	-2.05	119.65	122.62
4	B	402	NAD	O5B-PA-O1A	-2.03	100.91	108.94
4	B	402	NAD	N9A-C8A-N7A	-2.02	111.07	113.94
4	A	403	NAD	O5B-PA-O1A	-2.02	100.94	108.94
4	D	403	NAD	C2N-N1N-C1D	2.01	123.57	119.13

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FLC	CG-CB-CBC-OB1
2	A	401	FLC	CG-CB-CBC-OB2
2	A	401	FLC	OHB-CB-CBC-OB1
2	A	401	FLC	OHB-CB-CBC-OB2
2	A	401	FLC	CBC-CB-CG-CGC
2	A	401	FLC	OHB-CB-CG-CGC
2	C	401	FLC	CA-CB-CBC-OB2
2	D	401	FLC	CA-CB-CBC-OB1
2	D	401	FLC	CA-CB-CBC-OB2
2	D	401	FLC	OHB-CB-CBC-OB1
2	D	401	FLC	OHB-CB-CBC-OB2
2	E	402	FLC	OHB-CB-CBC-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	401	FLC	CA-CB-CBC-OB2
2	F	401	FLC	OHB-CB-CBC-OB1
2	F	401	FLC	OHB-CB-CBC-OB2
3	A	402	PE8	C2-C3-O4-C5
3	A	402	PE8	C5-C6-O7-C8
3	A	402	PE8	C14-C15-O16-C17
4	F	402	NAD	O4D-C4D-C5D-O5D
2	A	401	FLC	CA-CB-CG-CGC
3	D	402	PE8	C9-C8-O7-C6
4	C	402	NAD	O4D-C4D-C5D-O5D
4	E	403	NAD	O4D-C4D-C5D-O5D
2	E	401	FLC	CAC-CA-CB-OHB
3	D	402	PE8	C18-C17-O16-C15
3	A	402	PE8	O1-C2-C3-O4
2	F	401	FLC	CA-CB-CBC-OB1
2	E	401	FLC	CBC-CB-CG-CGC
3	A	402	PE8	O22-C23-C24-O25
3	D	402	PE8	O16-C17-C18-O19
3	D	402	PE8	O10-C11-C12-O13
2	F	401	FLC	CA-CB-CG-CGC
2	E	402	FLC	OHB-CB-CBC-OB1
2	C	401	FLC	CA-CB-CBC-OB1
3	D	402	PE8	O22-C23-C24-O25
4	A	403	NAD	O4D-C4D-C5D-O5D
4	C	402	NAD	C3D-C4D-C5D-O5D
2	D	401	FLC	CB-CA-CAC-OA1
2	B	401	FLC	CAC-CA-CB-OHB
2	B	401	FLC	CA-CB-CG-CGC
2	E	401	FLC	CA-CB-CG-CGC
4	E	403	NAD	C3D-C4D-C5D-O5D
4	F	402	NAD	C3D-C4D-C5D-O5D
2	D	401	FLC	CB-CA-CAC-OA2
3	A	402	PE8	C6-C5-O4-C3
3	D	402	PE8	C5-C6-O7-C8
3	D	402	PE8	C8-C9-O10-C11
4	B	402	NAD	O4B-C4B-C5B-O5B
4	A	403	NAD	C2B-C1B-N9A-C8A
2	C	401	FLC	CG-CB-CBC-OB2
2	E	402	FLC	CG-CB-CBC-OB1
2	E	402	FLC	CG-CB-CBC-OB2
2	B	401	FLC	CAC-CA-CB-CBC
2	E	401	FLC	OHB-CB-CG-CGC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	402	PE8	C21-C20-O19-C18
3	A	402	PE8	O7-C8-C9-O10
2	F	401	FLC	OHB-CB-CG-CGC
3	A	402	PE8	C20-C21-O22-C23
4	D	403	NAD	O4D-C4D-C5D-O5D
3	D	402	PE8	C14-C15-O16-C17
3	A	402	PE8	O13-C14-C15-O16
2	A	401	FLC	CA-CB-CBC-OB1
2	A	401	FLC	CA-CB-CBC-OB2
3	A	402	PE8	C18-C17-O16-C15
3	A	402	PE8	C12-C11-O10-C9
3	A	402	PE8	O19-C20-C21-O22
2	E	401	FLC	CAC-CA-CB-CBC
3	A	402	PE8	C9-C8-O7-C6
2	D	401	FLC	CB-CG-CGC-OG2
3	A	402	PE8	O4-C5-C6-O7
2	B	401	FLC	CBC-CB-CG-CGC
3	D	402	PE8	C24-C23-O22-C21
2	B	401	FLC	CG-CB-CBC-OB1
2	C	401	FLC	CG-CB-CBC-OB1
2	E	402	FLC	CA-CB-CBC-OB2
4	A	403	NAD	O4B-C1B-N9A-C8A
2	A	401	FLC	CB-CG-CGC-OG2
2	D	401	FLC	CB-CG-CGC-OG1
2	D	401	FLC	CAC-CA-CB-OHB
4	C	402	NAD	O4B-C4B-C5B-O5B
3	D	402	PE8	O4-C5-C6-O7
4	C	402	NAD	C2B-C1B-N9A-C8A
4	E	403	NAD	C2B-C1B-N9A-C8A
2	C	401	FLC	OHB-CB-CBC-OB1
2	C	401	FLC	OHB-CB-CBC-OB2
2	E	401	FLC	CB-CA-CAC-OA1
4	A	403	NAD	O4B-C4B-C5B-O5B
4	D	403	NAD	C3D-C4D-C5D-O5D
2	A	401	FLC	CB-CG-CGC-OG1
2	E	401	FLC	CB-CA-CAC-OA2
2	A	401	FLC	CB-CA-CAC-OA1
3	D	402	PE8	O13-C14-C15-O16
3	D	402	PE8	C2-C3-O4-C5
2	E	401	FLC	CB-CG-CGC-OG1
2	B	401	FLC	OHB-CB-CG-CGC
2	A	401	FLC	CB-CA-CAC-OA2

Continued on next page...

Continued from previous page...

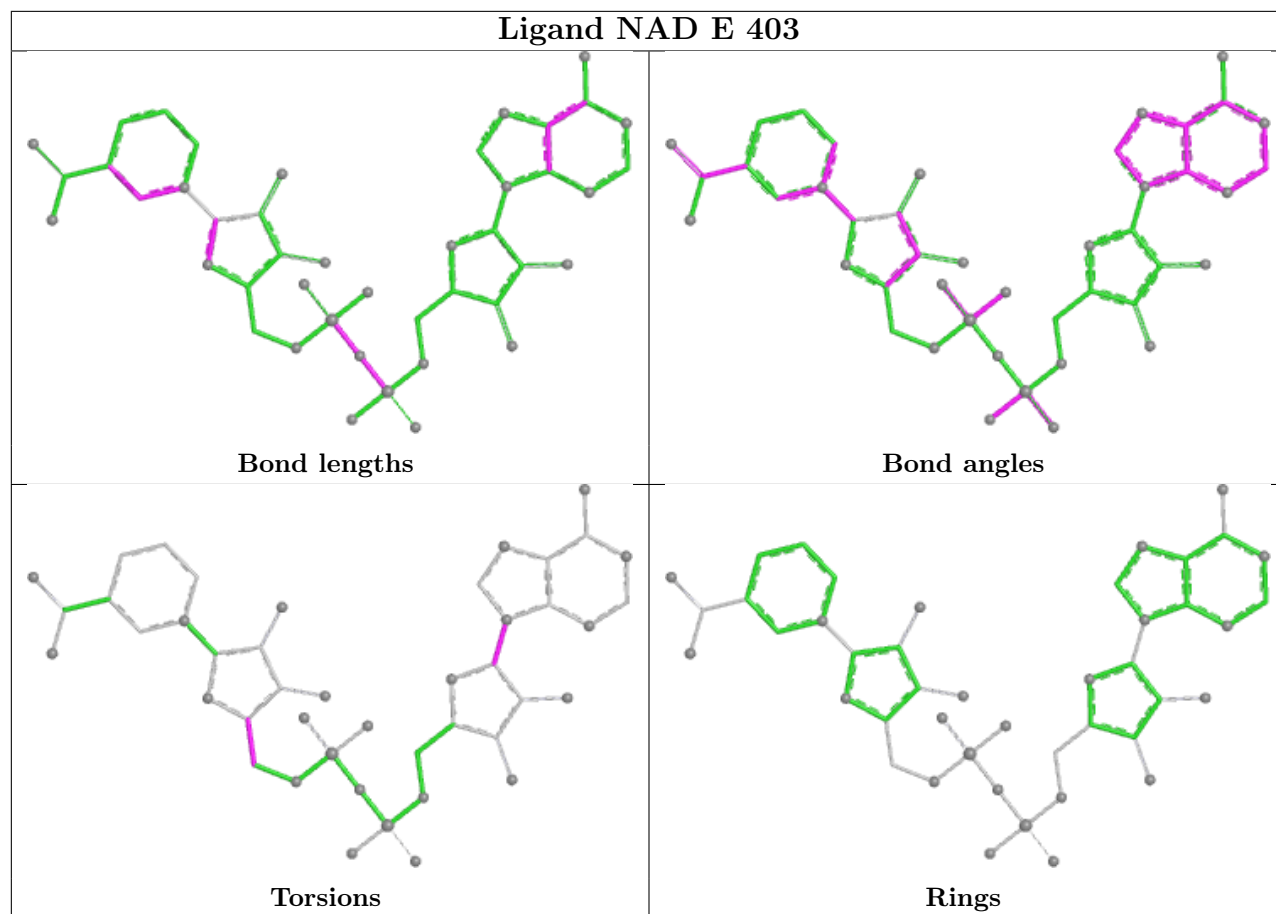
Mol	Chain	Res	Type	Atoms
4	A	403	NAD	C3D-C4D-C5D-O5D

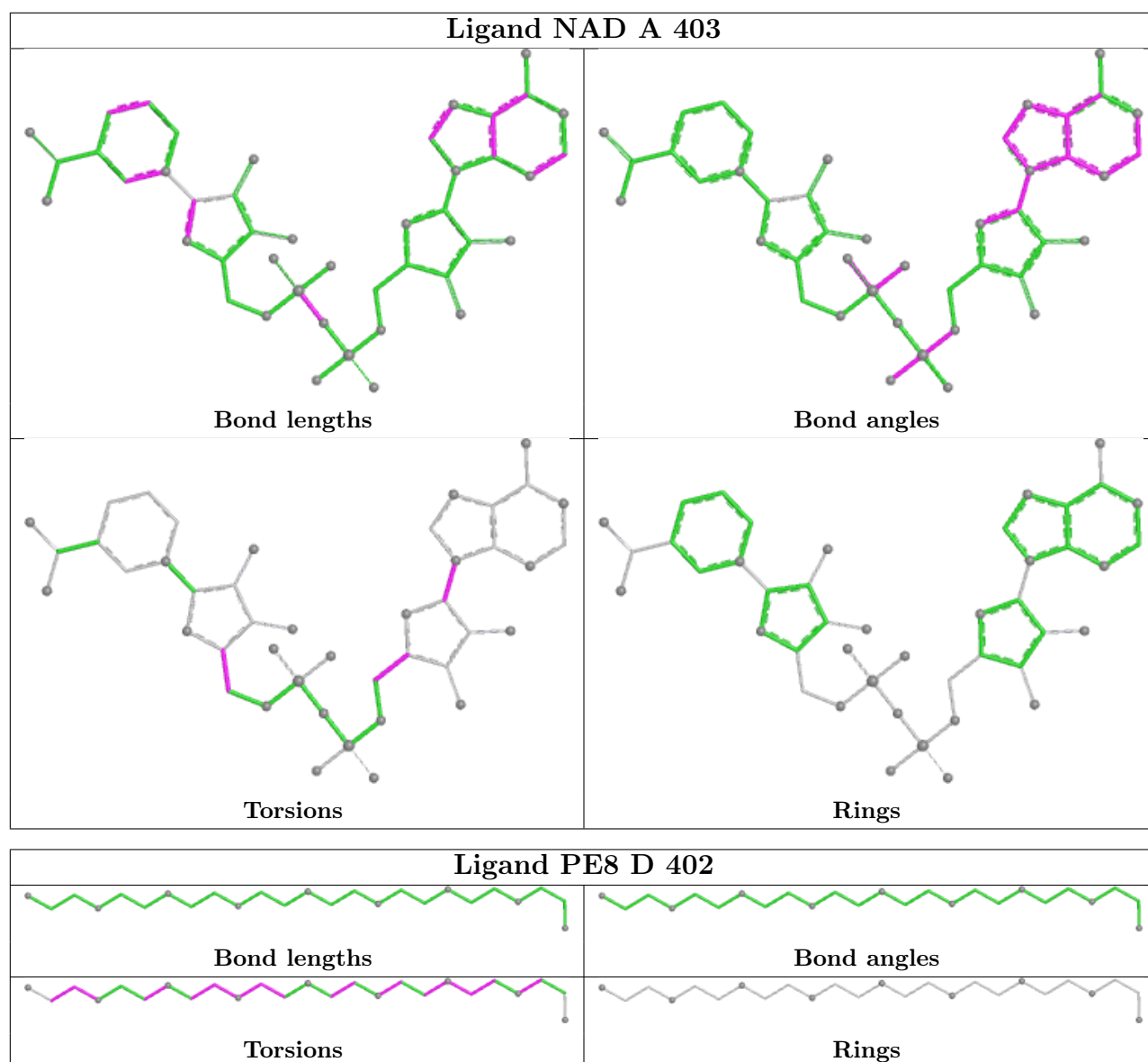
There are no ring outliers.

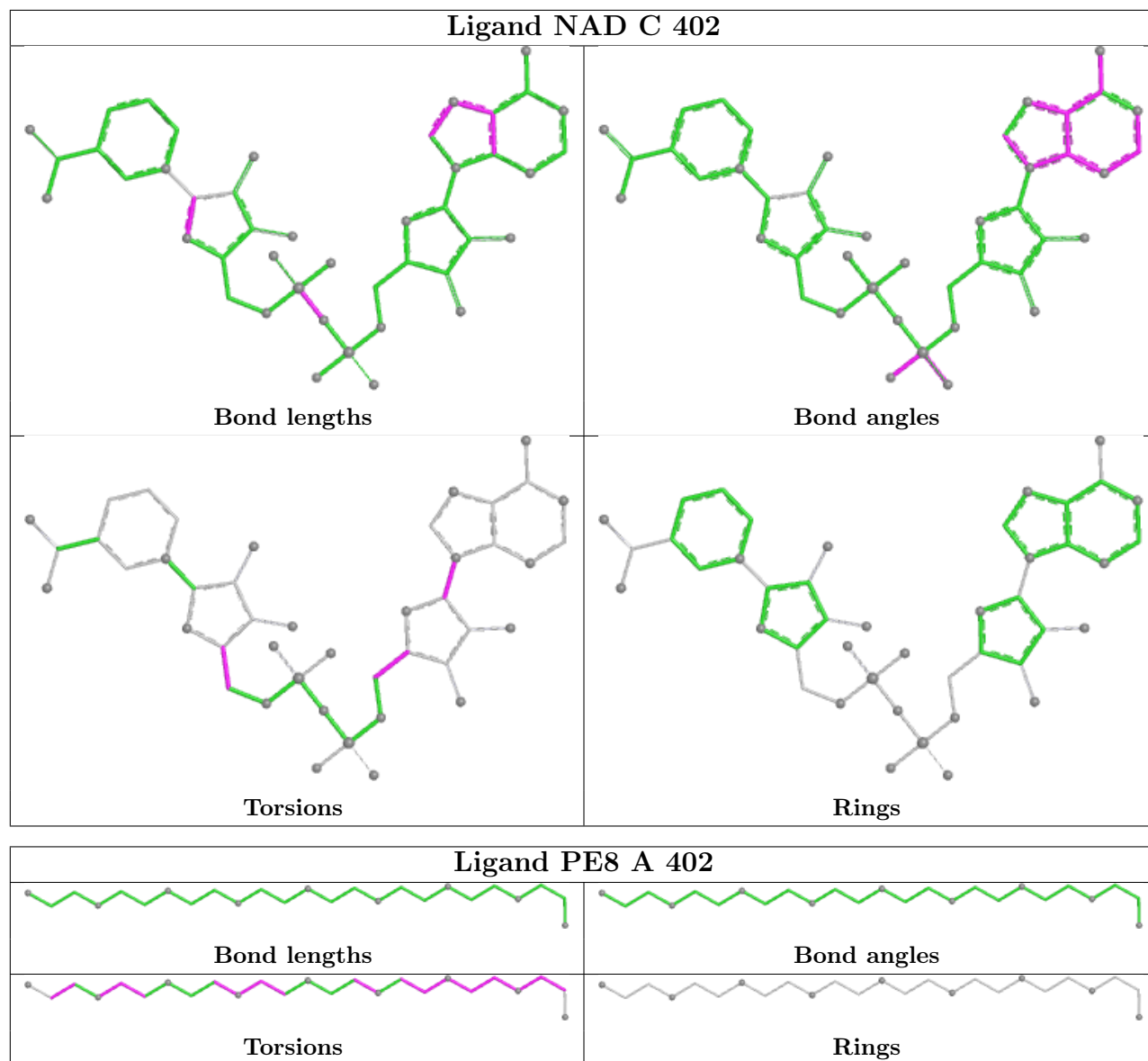
15 monomers are involved in 65 short contacts:

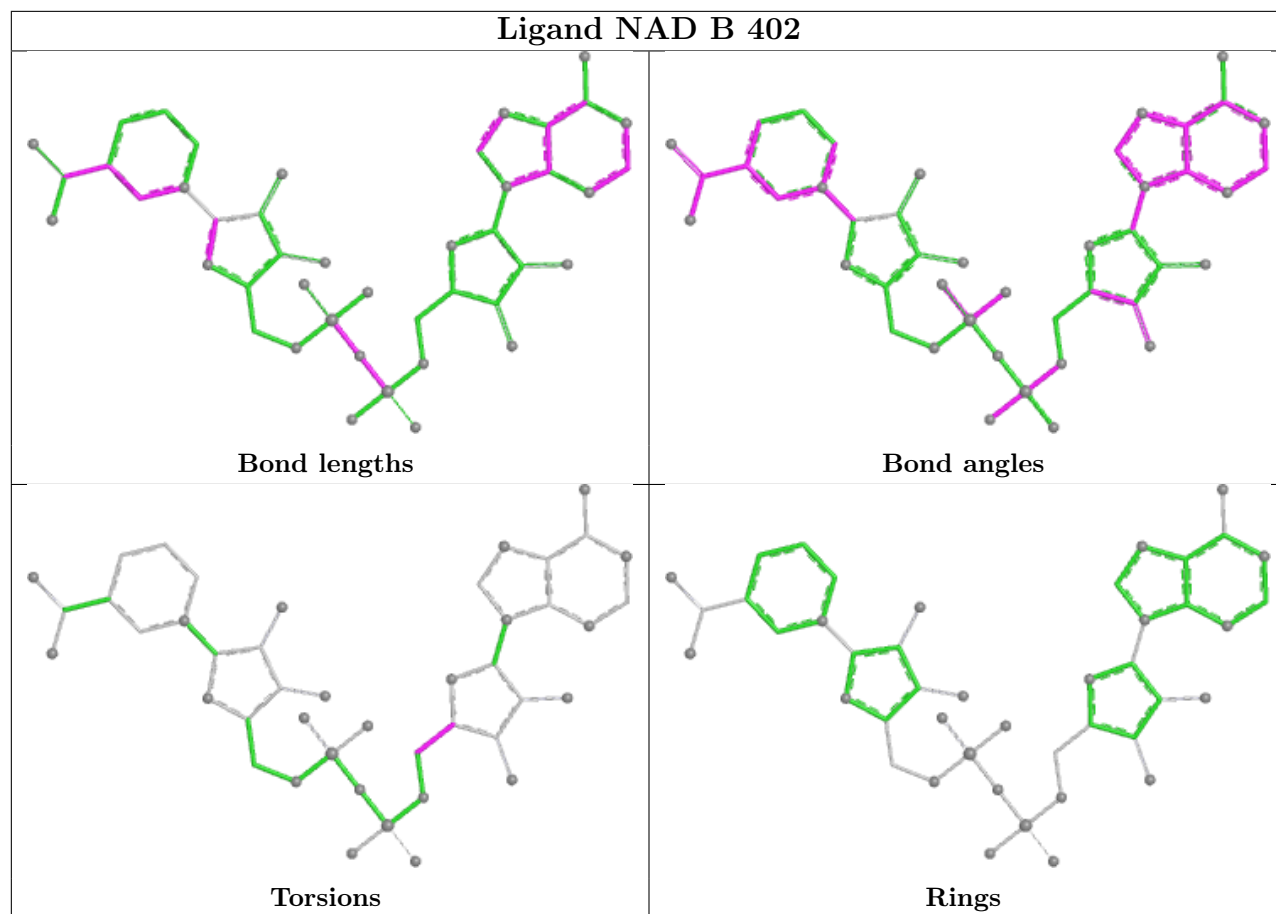
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	FLC	3	0
2	A	401	FLC	3	0
4	E	403	NAD	6	0
4	A	403	NAD	5	0
2	E	402	FLC	1	0
3	D	402	PE8	10	0
4	C	402	NAD	4	0
3	A	402	PE8	13	0
4	B	402	NAD	7	0
2	F	401	FLC	3	0
4	F	402	NAD	8	0
2	E	401	FLC	3	0
2	C	401	FLC	1	0
4	D	403	NAD	4	0
2	D	401	FLC	1	0

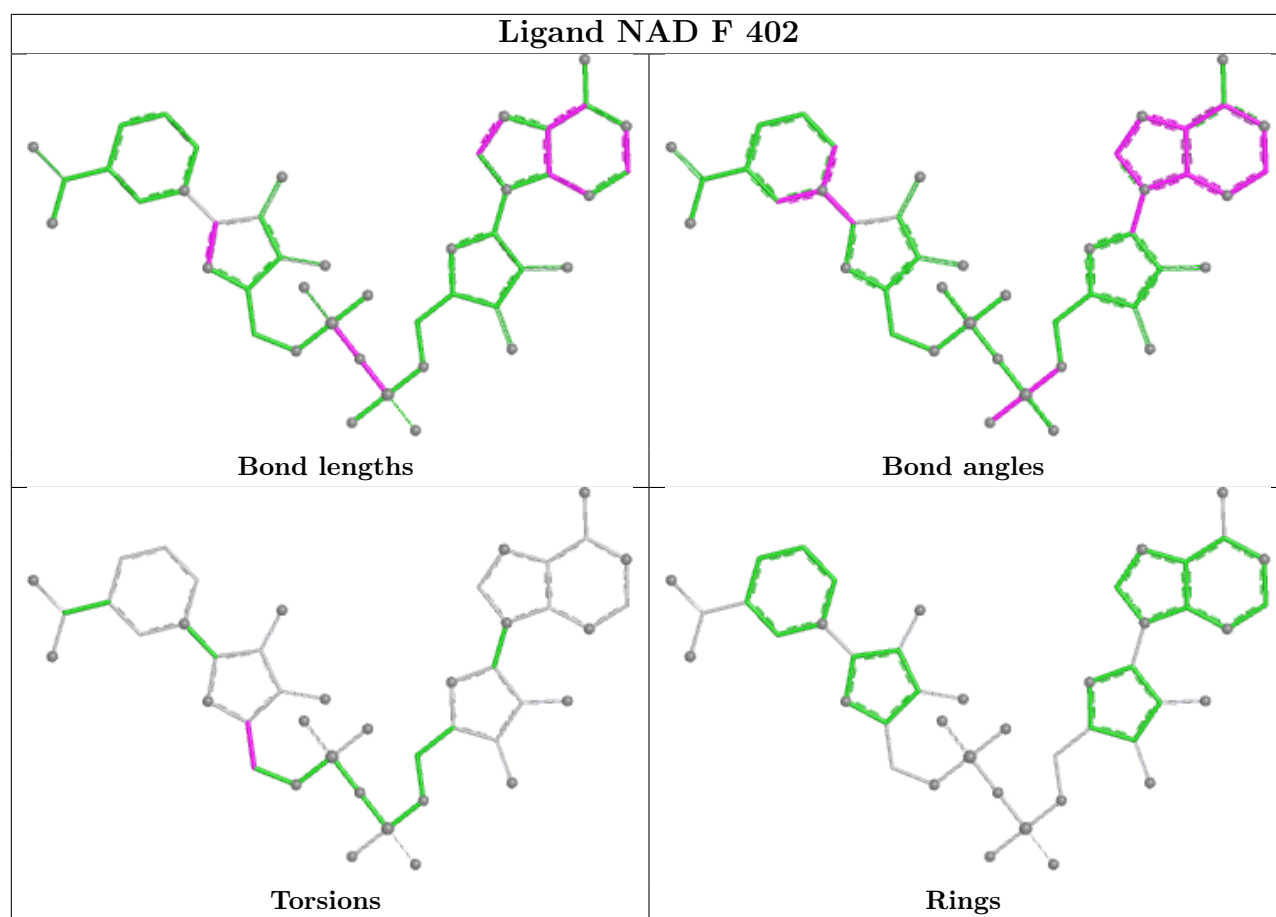
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

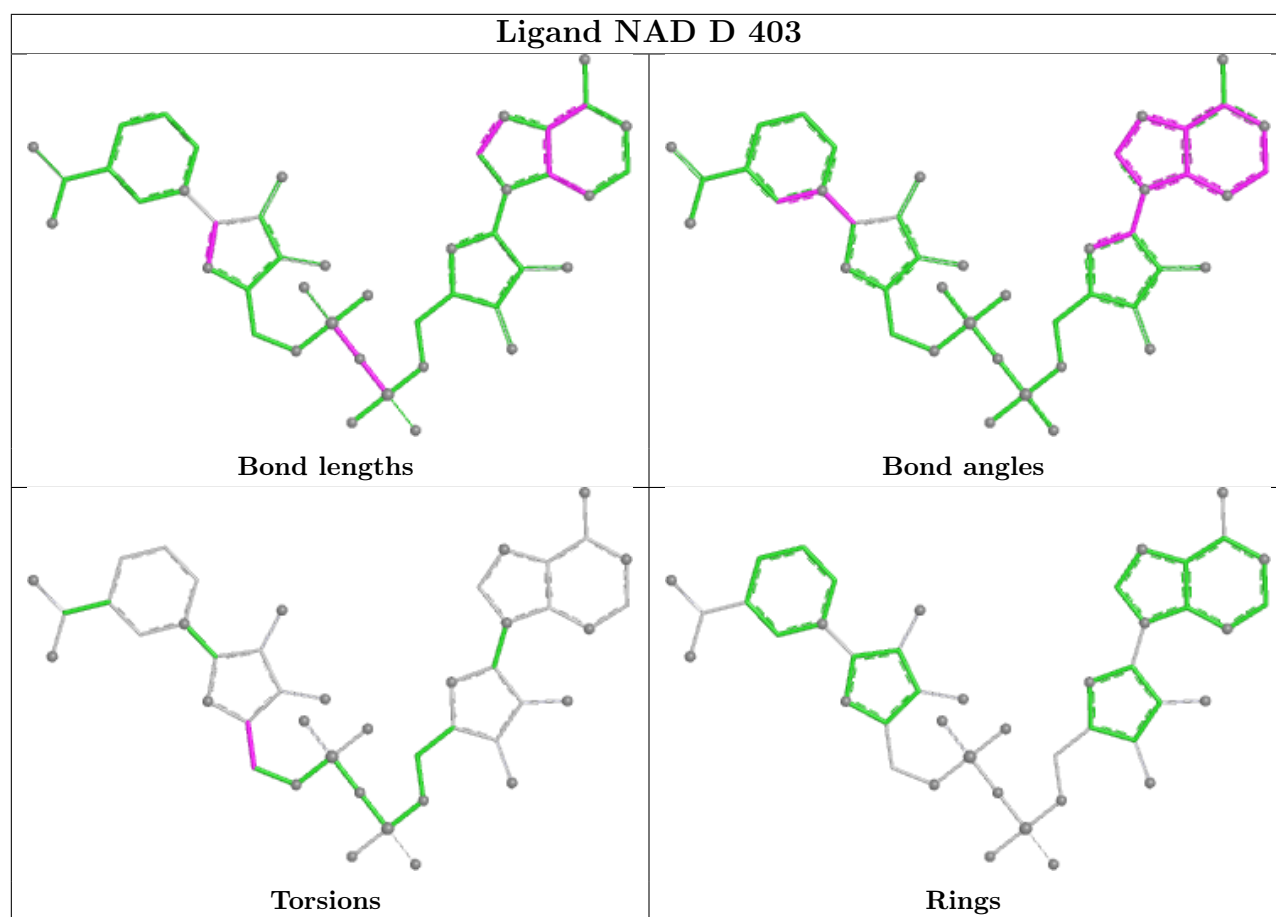












5.7 Other polymers [i](#)

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	306/345 (88%)	0.07	3 (0%) 79 81	21, 34, 57, 75	0
1	B	306/345 (88%)	0.21	9 (2%) 53 56	23, 37, 56, 69	0
1	C	306/345 (88%)	0.21	7 (2%) 61 63	20, 37, 57, 81	0
1	D	307/345 (88%)	0.39	9 (2%) 53 56	26, 42, 61, 96	0
1	E	304/345 (88%)	0.20	6 (1%) 65 67	21, 36, 55, 71	0
1	F	307/345 (88%)	0.40	12 (3%) 43 46	25, 41, 62, 90	0
All	All	1836/2070 (88%)	0.25	46 (2%) 58 61	20, 38, 59, 96	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	334	LEU	5.3
1	D	334	LEU	4.5
1	F	290	PHE	4.4
1	A	334	LEU	4.0
1	F	334	LEU	3.9
1	B	334	LEU	3.3
1	F	200	PRO	3.0
1	E	67	ASP	3.0
1	B	300	ARG	2.9
1	E	62	GLY	2.6
1	C	102	ALA	2.6
1	B	199	LEU	2.5
1	C	198	ALA	2.5
1	D	66	ARG	2.5
1	B	290	PHE	2.5
1	F	300	ARG	2.5
1	E	290	PHE	2.4
1	B	227	ARG	2.4
1	F	285	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	69	ASN	2.4
1	D	67	ASP	2.4
1	C	333	LYS	2.4
1	A	227	ARG	2.4
1	F	229	ALA	2.3
1	E	108	PRO	2.3
1	B	287	LYS	2.3
1	F	151	THR	2.3
1	B	128	GLN	2.3
1	A	62	GLY	2.3
1	F	66	ARG	2.3
1	E	198	ALA	2.2
1	B	103	VAL	2.2
1	D	117	ARG	2.2
1	D	62	GLY	2.2
1	F	100	LEU	2.2
1	C	67	ASP	2.2
1	F	67	ASP	2.2
1	C	59	LYS	2.1
1	F	294	ILE	2.1
1	B	117	ARG	2.1
1	F	227	ARG	2.1
1	E	302	ILE	2.1
1	D	300	ARG	2.1
1	D	333	LYS	2.0
1	D	102	ALA	2.0
1	D	68	GLY	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,

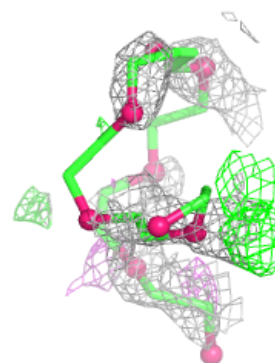
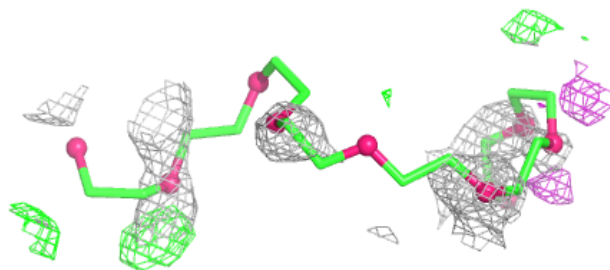
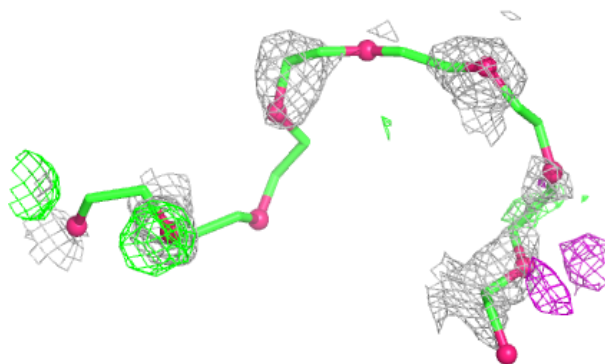
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PE8	D	402	25/25	0.68	0.32	80,93,108,108	0
2	FLC	F	401	13/13	0.70	0.21	59,68,74,75	0
2	FLC	D	401	13/13	0.70	0.21	65,70,72,74	0
3	PE8	A	402	25/25	0.72	0.26	60,72,74,76	0
2	FLC	C	401	13/13	0.81	0.21	77,82,85,85	0
2	FLC	A	401	13/13	0.83	0.18	64,65,69,72	0
2	FLC	E	401	13/13	0.84	0.18	68,75,79,80	0
2	FLC	E	402	13/13	0.85	0.15	63,67,69,70	0
2	FLC	B	401	13/13	0.86	0.17	77,82,87,89	0
4	NAD	A	403	44/44	0.93	0.08	27,36,43,49	0
4	NAD	D	403	44/44	0.93	0.09	35,43,58,66	0
4	NAD	E	403	44/44	0.93	0.09	27,34,44,49	0
4	NAD	F	402	44/44	0.93	0.09	24,37,43,49	0
4	NAD	B	402	44/44	0.94	0.08	25,37,45,47	0
4	NAD	C	402	44/44	0.95	0.08	28,39,59,64	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.

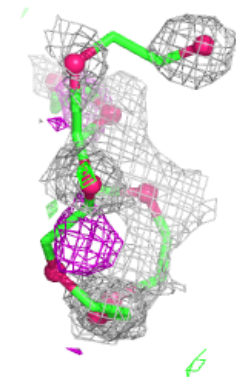
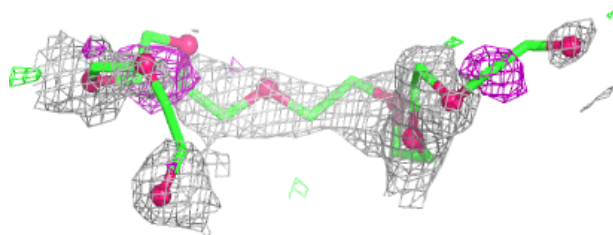
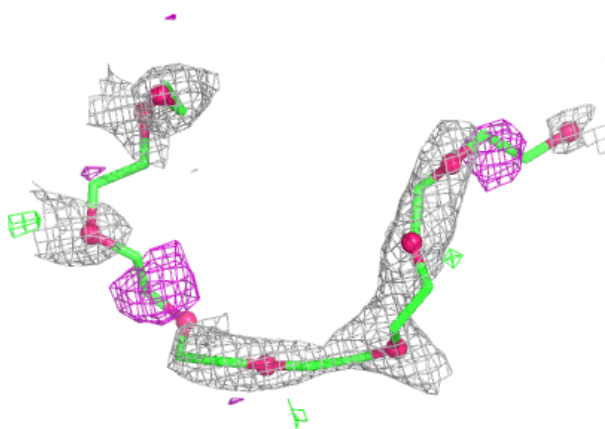
Electron density around PE8 D 402:

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

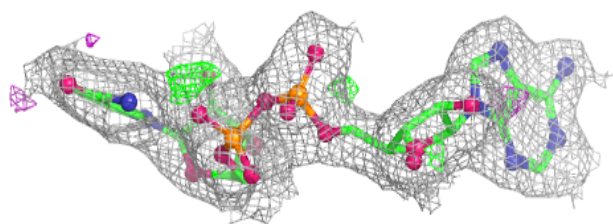
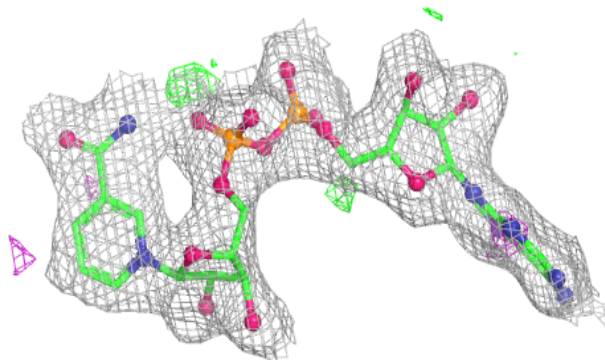


Electron density around PE8 A 402:

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

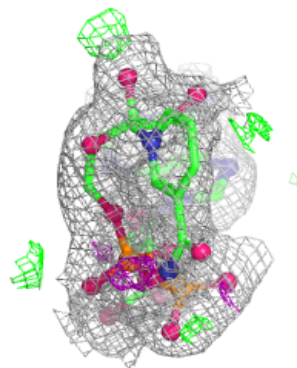
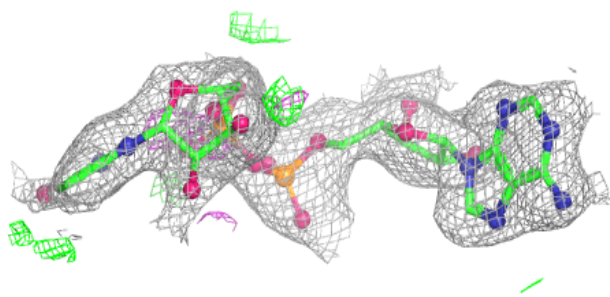
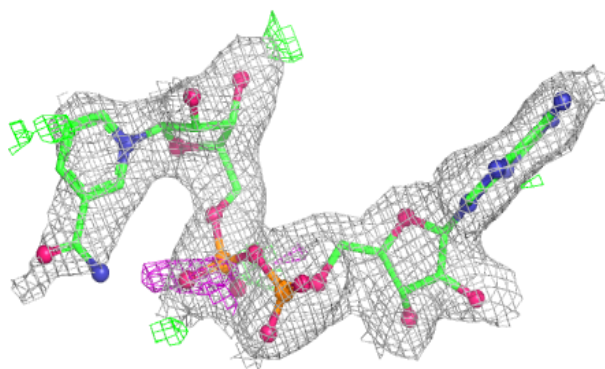
**Electron density around NAD A 403:**

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

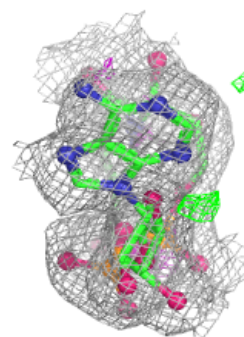
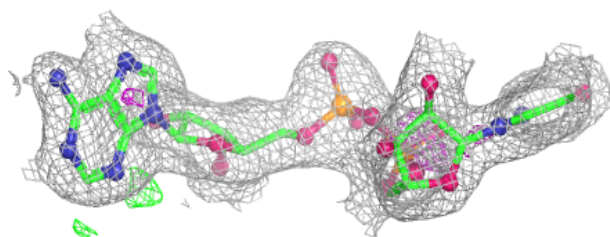
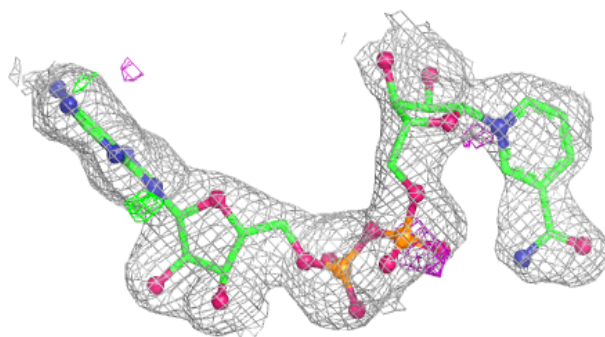


Electron density around NAD D 403:

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

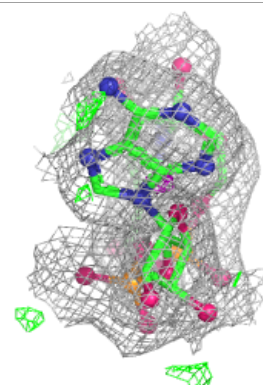
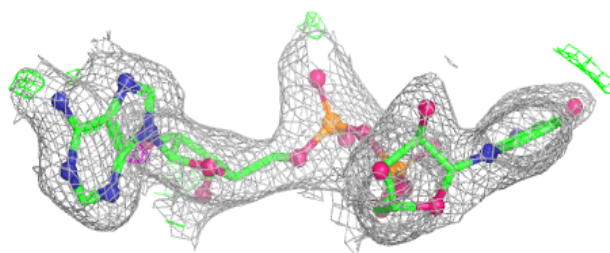
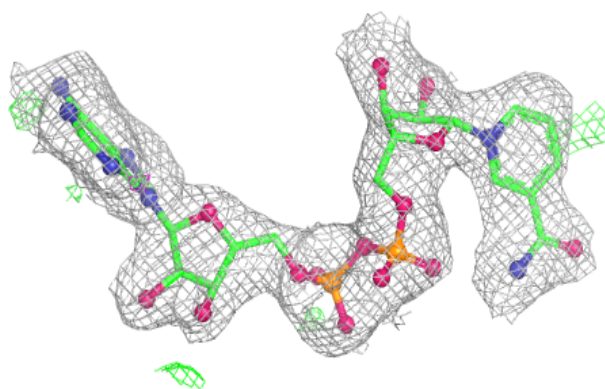
**Electron density around NAD E 403:**

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

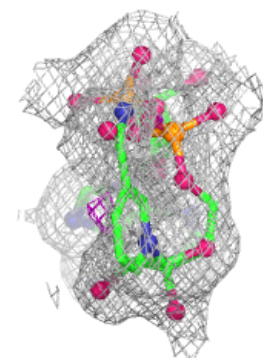
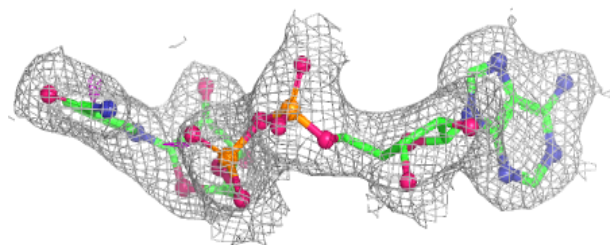
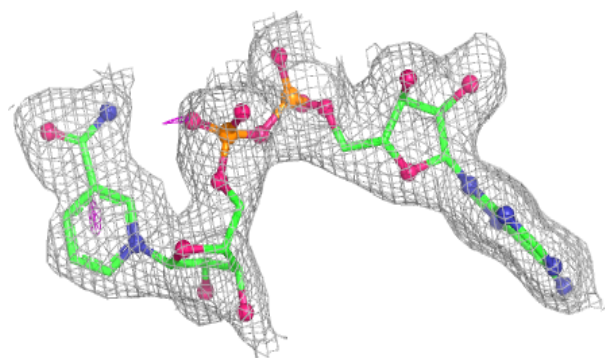


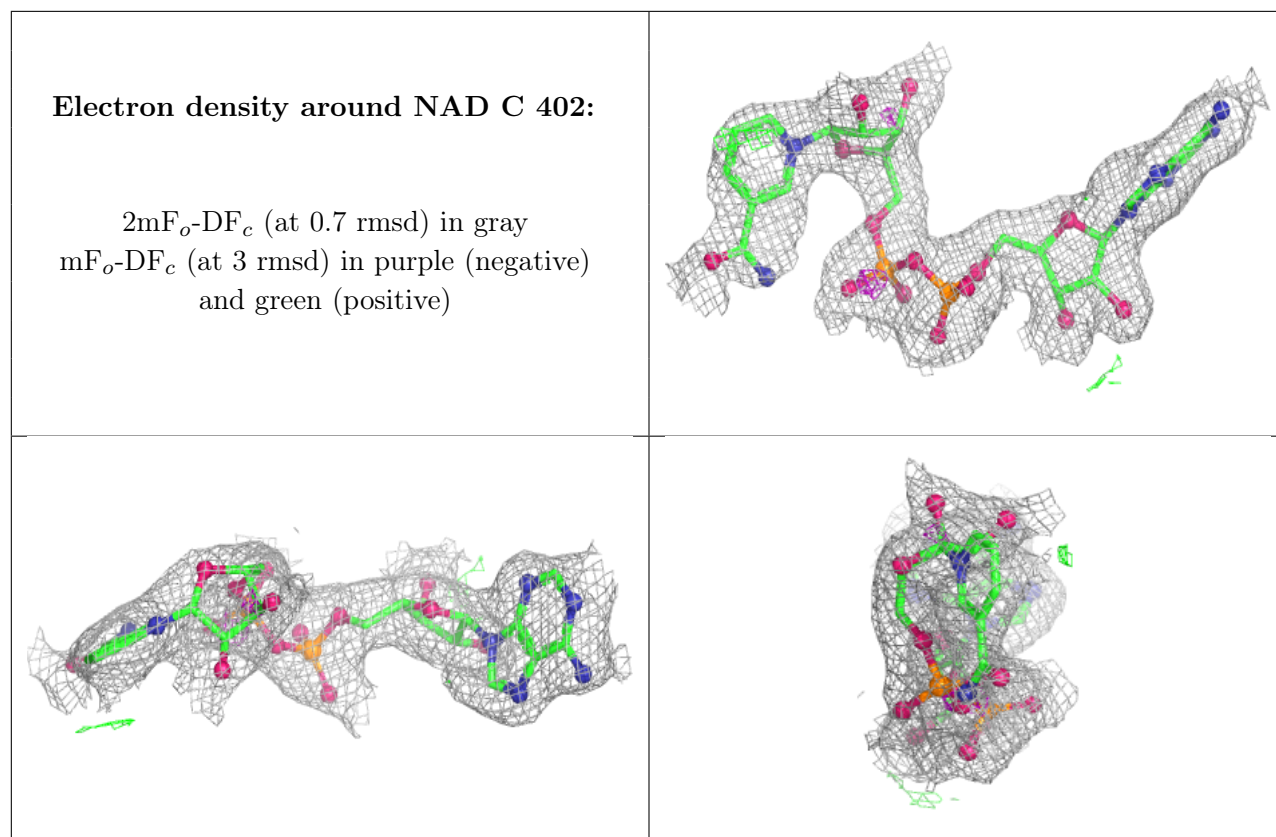
Electron density around NAD F 402:

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

**Electron density around NAD B 402:**

$2mF_o-DF_c$ (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.