



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:42 AM UTC

PDB ID : 7XR9 / pdb_00007xr9
Title : Crystal structure of DgpA with glucose
Authors : Ma, W.; He, P.
Deposited on : 2022-05-09
Resolution : 2.42 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:

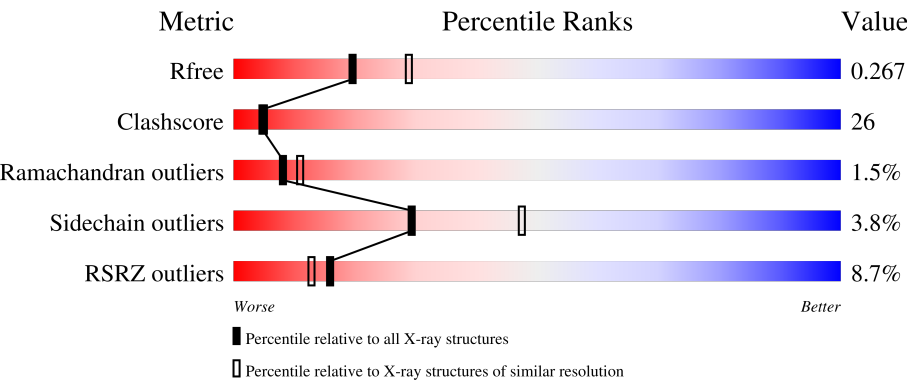
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	367	17% 46%39%8%6%
1	B	367	3% 69%25%
1	C	367	6% 61%32%5%
1	D	367	11% 51%39%5%
1	E	367	4% 63%27%5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	367	 10% 46% 40% 9% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16422 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.

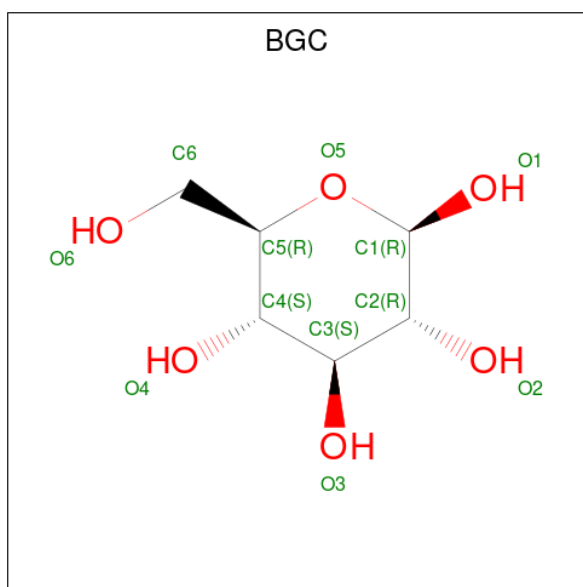
- Molecule 1 is a protein called DgpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2574	1612	443	503	16			
1	B	354	Total	C	N	O	S	0	0	0
			2687	1687	463	520	17			
1	C	350	Total	C	N	O	S	0	0	0
			2674	1680	460	517	17			
1	D	350	Total	C	N	O	S	0	0	0
			2639	1658	452	513	16			
1	E	353	Total	C	N	O	S	0	0	0
			2679	1682	461	520	16			
1	F	350	Total	C	N	O	S	0	0	0
			2621	1652	437	516	16			

There are 6 discrepancies between the modelled and reference sequences:

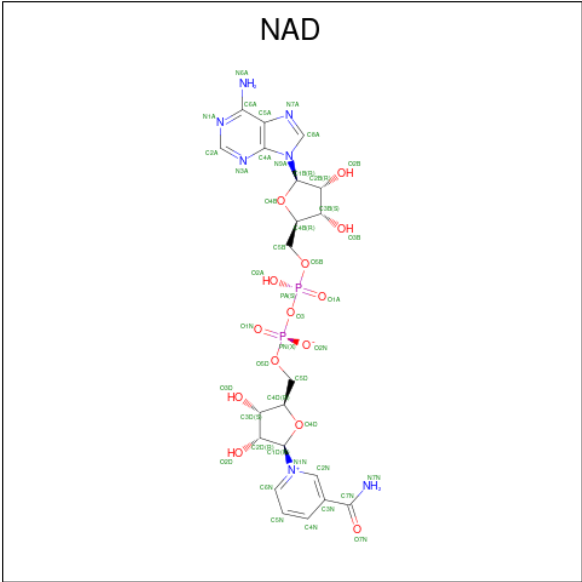
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A3Q9WWX8
B	0	GLY	-	expression tag	UNP A0A3Q9WWX8
C	0	GLY	-	expression tag	UNP A0A3Q9WWX8
D	0	GLY	-	expression tag	UNP A0A3Q9WWX8
E	0	GLY	-	expression tag	UNP A0A3Q9WWX8
F	0	GLY	-	expression tag	UNP A0A3Q9WWX8

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		
2	E	1	Total	C	O	0	0
			12	6	6		
2	F	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

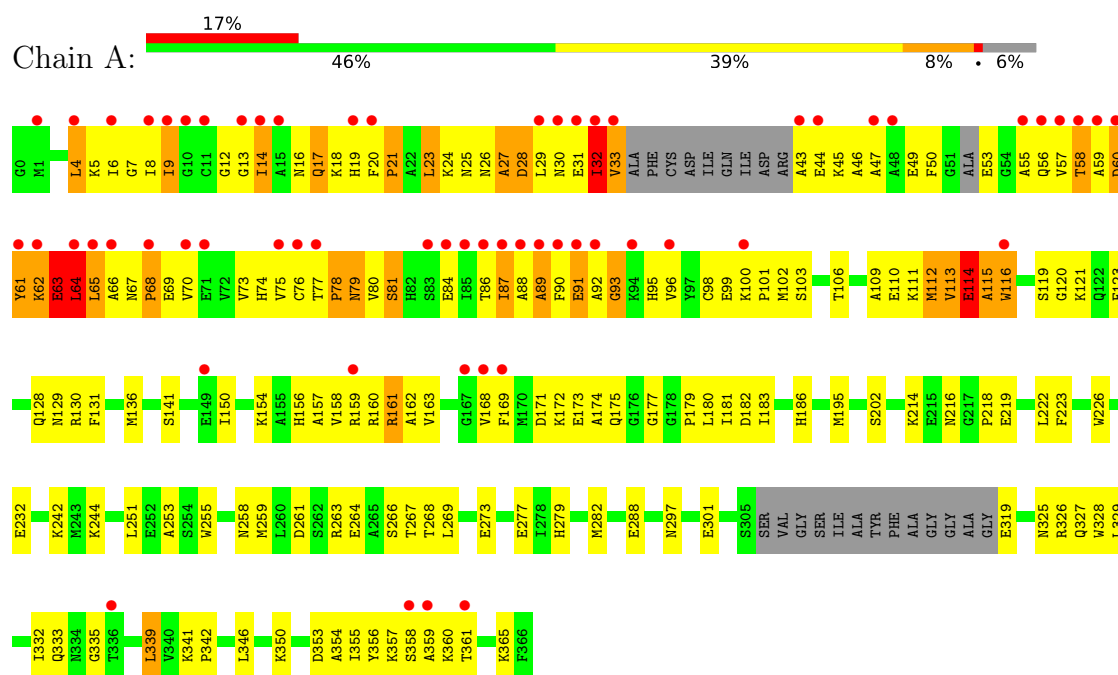
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	53	Total	O	0	0
			53	53		
4	C	31	Total	O	0	0
			31	31		
4	D	30	Total	O	0	0
			30	30		
4	E	40	Total	O	0	0
			40	40		
4	F	37	Total	O	0	0
			37	37		

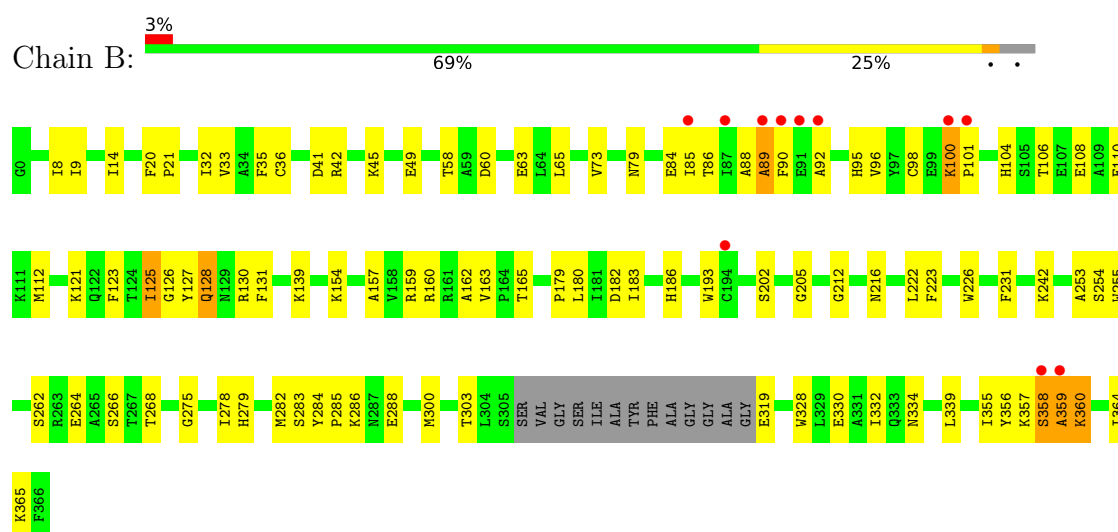
3 Residue-property plots [i](#)

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.

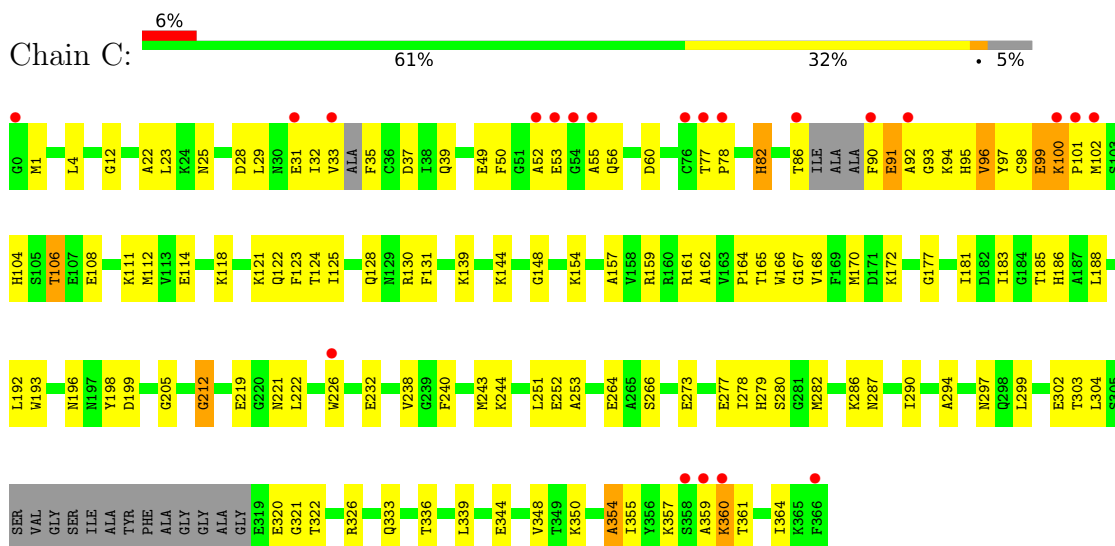
• Molecule 1: DgpA



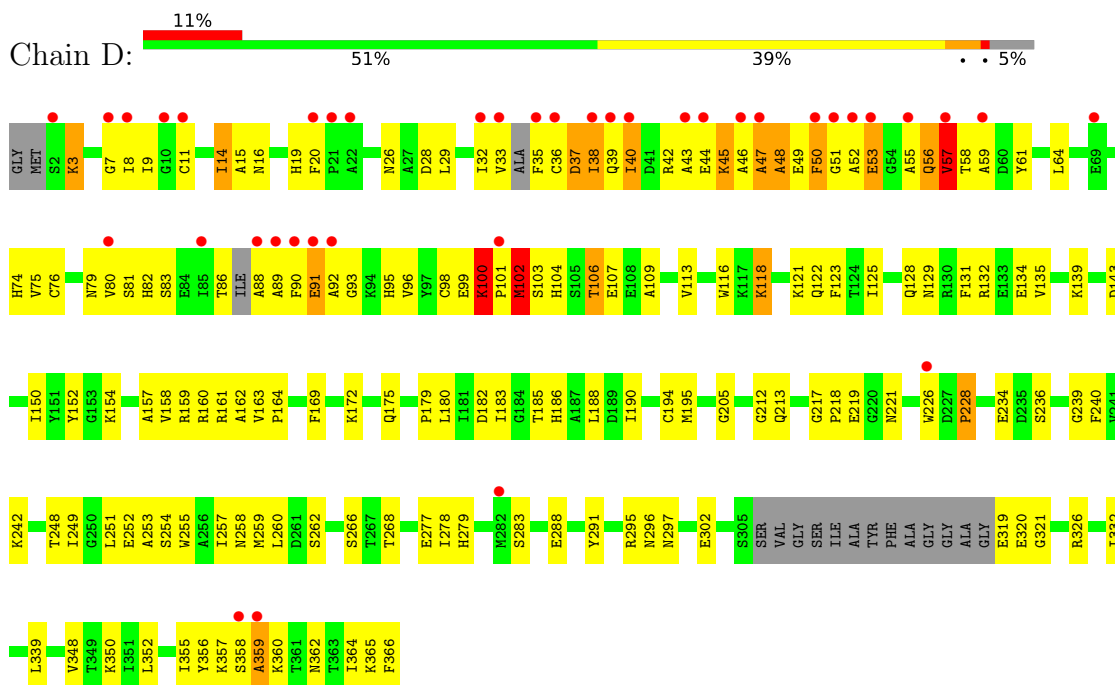
• Molecule 1: DgpA



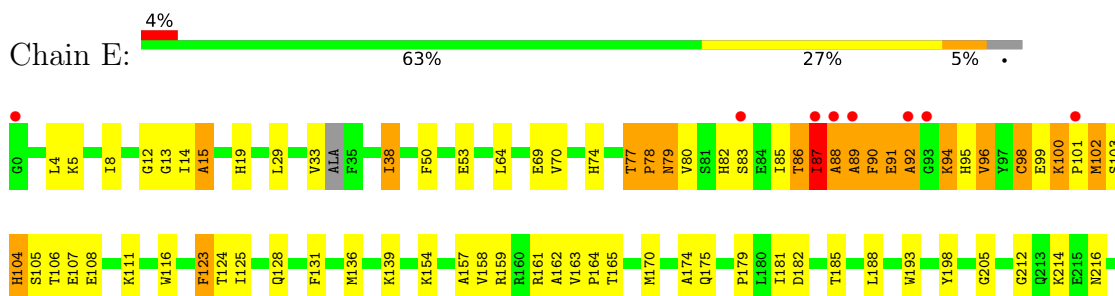
- Molecule 1: DgpA

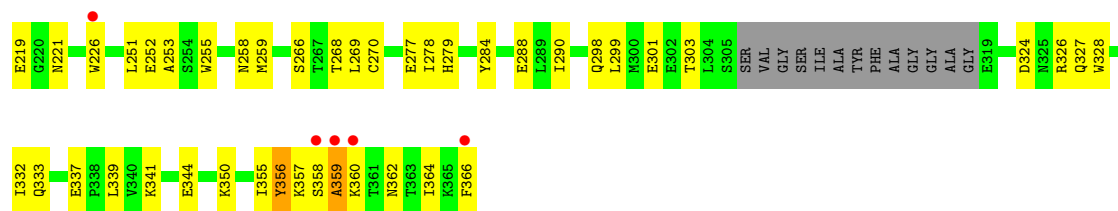


- Molecule 1: DgpA

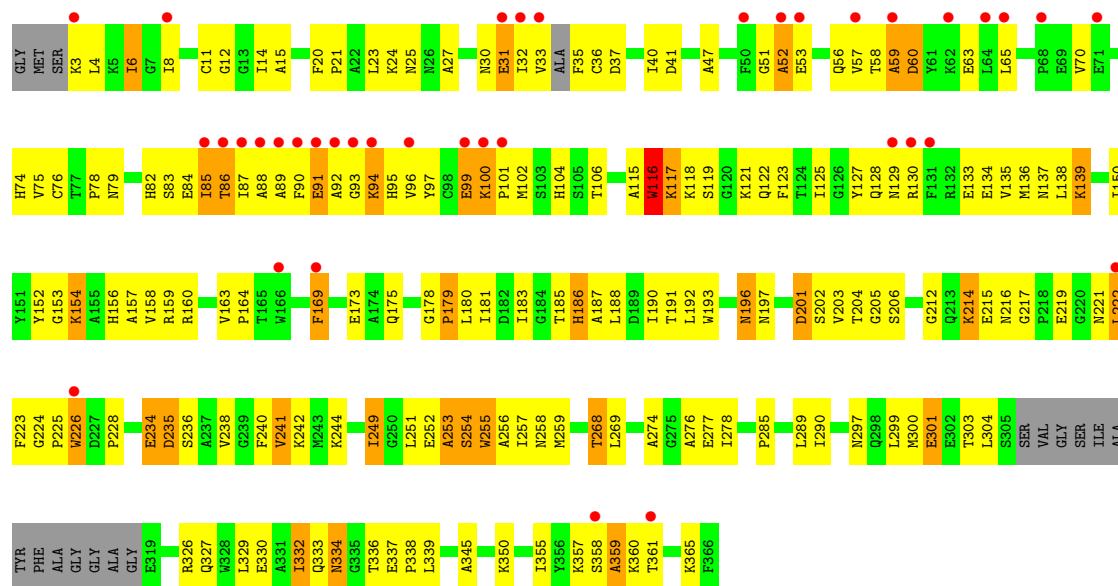


- Molecule 1: DgpA





● Molecule 1: DgpA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.33Å 128.99Å 204.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.50 – 2.42 22.50 – 2.42	Depositor EDS
% Data completeness (in resolution range)	100.0 (22.50-2.42) 90.9 (22.50-2.42)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.222 , 0.267 0.237 , 0.267	Depositor DCC
R_{free} test set	4799 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16422	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: BGC, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	6/2621 (0.2%)	1.20	34/3548 (1.0%)
1	B	0.67	6/2738 (0.2%)	0.85	8/3703 (0.2%)
1	C	0.71	4/2723 (0.1%)	0.83	7/3677 (0.2%)
1	D	0.86	8/2688 (0.3%)	1.06	14/3640 (0.4%)
1	E	0.73	10/2729 (0.4%)	0.89	15/3691 (0.4%)
1	F	1.46	44/2671 (1.6%)	1.40	29/3621 (0.8%)
All	All	0.91	78/16170 (0.5%)	1.06	107/21880 (0.5%)

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	ASN	C-N	-11.56	1.26	1.34
1	D	57	VAL	C-O	-8.40	1.14	1.24
1	E	78	PRO	C-O	-8.21	1.13	1.23
1	F	179	PRO	C-O	-7.56	1.14	1.24
1	F	285	PRO	C-O	-7.55	1.15	1.24
1	F	225	PRO	C-O	-7.32	1.15	1.23
1	F	269	LEU	C-O	-7.11	1.15	1.24
1	B	125	ILE	C-O	-7.07	1.15	1.24
1	A	46	ALA	C-O	-7.01	1.16	1.24
1	E	50	PHE	C-O	-7.01	1.15	1.24
1	F	56	GLN	C-O	-6.92	1.15	1.23
1	F	252	GLU	C-O	-6.77	1.16	1.24
1	F	274	ALA	C-O	-6.68	1.15	1.24
1	F	138	LEU	C-O	-6.47	1.16	1.24
1	F	276	ALA	C-O	-6.44	1.16	1.23
1	C	243	MET	C-O	-6.37	1.15	1.23
1	F	238	VAL	C-O	-6.31	1.17	1.24
1	F	187	ALA	C-O	-6.27	1.16	1.24
1	F	139	LYS	C-O	-6.25	1.16	1.24
1	E	98	CYS	C-O	-6.24	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	253	ALA	C-O	-6.23	1.17	1.23
1	F	197	ASN	C-O	-6.21	1.16	1.23
1	D	364	ILE	C-O	-6.17	1.17	1.24
1	F	154	LYS	C-O	-6.08	1.16	1.24
1	F	205	GLY	C-O	-6.05	1.17	1.24
1	F	301	GLU	C-O	-6.00	1.17	1.23
1	F	236	SER	C-O	-5.89	1.16	1.23
1	F	188	LEU	C-O	-5.87	1.17	1.24
1	F	249	ILE	C-O	-5.81	1.17	1.24
1	E	77	THR	C-O	-5.77	1.15	1.23
1	F	242	LYS	C-O	-5.74	1.17	1.24
1	D	58	THR	C-O	-5.72	1.16	1.23
1	E	15	ALA	C-O	-5.70	1.17	1.24
1	F	181	ILE	C-O	-5.69	1.18	1.24
1	A	242	LYS	C-O	-5.68	1.17	1.24
1	F	6	ILE	C-N	5.68	1.38	1.33
1	F	289	LEU	C-O	-5.65	1.17	1.24
1	F	241	VAL	C-O	-5.62	1.18	1.24
1	F	300	MET	C-O	-5.62	1.16	1.23
1	F	204	THR	C-O	-5.61	1.16	1.24
1	F	133	GLU	C-O	-5.58	1.17	1.24
1	F	235	ASP	C-O	-5.49	1.17	1.24
1	F	78	PRO	N-CA	-5.49	1.40	1.47
1	F	136	MET	C-O	-5.49	1.17	1.24
1	F	206	SER	C-O	-5.48	1.17	1.23
1	F	228	PRO	C-O	-5.47	1.16	1.24
1	F	192	LEU	C-O	-5.45	1.17	1.24
1	E	12	GLY	C-O	-5.45	1.18	1.24
1	F	201	ASP	C-O	-5.44	1.16	1.24
1	B	128	GLN	C-O	-5.37	1.17	1.24
1	F	277	GLU	C-O	-5.36	1.17	1.23
1	F	152	TYR	C-O	-5.36	1.17	1.23
1	C	106	THR	C-O	-5.35	1.17	1.24
1	E	99	GLU	C-O	-5.35	1.16	1.23
1	B	126	GLY	C-O	-5.34	1.16	1.23
1	D	103	SER	C-O	-5.29	1.17	1.23
1	E	13	GLY	C-O	-5.28	1.17	1.23
1	D	83	SER	C-O	-5.25	1.18	1.24
1	B	364	ILE	C-O	-5.25	1.18	1.24
1	D	221	ASN	C-O	-5.22	1.17	1.23
1	C	97	TYR	C-O	-5.22	1.18	1.24
1	A	301	GLU	C-O	-5.22	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	102	MET	C-O	-5.21	1.17	1.24
1	F	290	ILE	C-O	-5.20	1.18	1.24
1	A	21	PRO	C-O	-5.19	1.17	1.24
1	E	85	ILE	CA-CB	-5.17	1.47	1.54
1	F	234	GLU	C-O	-5.16	1.17	1.23
1	A	355	ILE	C-O	-5.12	1.18	1.24
1	F	186	HIS	C-O	-5.11	1.18	1.24
1	F	225	PRO	N-CA	-5.11	1.41	1.46
1	B	242	LYS	C-O	-5.09	1.17	1.24
1	F	254	SER	C-O	-5.08	1.17	1.23
1	C	354	ALA	C-O	-5.05	1.17	1.24
1	F	191	THR	C-O	-5.04	1.18	1.24
1	A	244	LYS	C-O	-5.03	1.17	1.24
1	D	228	PRO	C-O	-5.03	1.17	1.24
1	E	356	TYR	C-O	-5.02	1.18	1.24
1	F	251	LEU	C-O	-5.01	1.17	1.23

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	359	ALA	N-CA-C	-11.12	99.16	113.17
1	B	359	ALA	N-CA-C	-9.51	101.61	113.02
1	F	255	TRP	N-CA-C	-9.06	102.74	113.88
1	F	359	ALA	N-CA-C	-8.95	100.32	112.94
1	A	65	LEU	N-CA-C	-8.52	101.90	112.47
1	A	53	GLU	CB-CG-CD	8.26	126.64	112.60
1	E	360	LYS	N-CA-C	-8.23	102.80	113.17
1	A	114	GLU	CA-C-N	-8.00	109.75	120.54
1	A	114	GLU	C-N-CA	-8.00	109.75	120.54
1	A	45	LYS	CA-C-N	7.79	130.57	120.44
1	A	45	LYS	C-N-CA	7.79	130.57	120.44
1	E	359	ALA	N-CA-C	-7.72	104.28	112.93
1	F	360	LYS	N-CA-C	-7.69	103.47	112.92
1	A	79	ASN	CA-C-N	-7.57	109.68	120.42
1	A	79	ASN	C-N-CA	-7.57	109.68	120.42
1	F	156	HIS	CA-CB-CG	7.37	121.17	113.80
1	F	59	ALA	N-CA-C	-7.37	104.31	113.38
1	A	32	ILE	N-CA-CB	-7.31	104.01	111.90
1	F	222	LEU	N-CA-C	-7.27	100.95	110.33
1	A	25	ASN	N-CA-C	-7.24	103.71	112.54
1	A	335	GLY	CA-C-N	-7.23	109.73	123.32
1	A	335	GLY	C-N-CA	-7.23	109.73	123.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	PHE	CA-CB-CG	7.21	121.01	113.80
1	E	104	HIS	N-CA-C	-7.17	104.50	113.18
1	C	212	GLY	CA-C-N	-6.90	112.30	122.86
1	C	212	GLY	C-N-CA	-6.90	112.30	122.86
1	F	201	ASP	CA-CB-CG	6.90	119.50	112.60
1	F	137	ASN	CA-CB-CG	6.88	119.48	112.60
1	F	116	TRP	N-CA-C	-6.87	102.91	112.45
1	A	9	ILE	N-CA-C	6.79	116.92	110.74
1	F	358	SER	N-CA-C	-6.73	100.27	110.70
1	D	57	VAL	N-CA-C	6.67	123.22	109.34
1	E	79	ASN	CA-CB-CG	6.61	119.21	112.60
1	D	48	ALA	N-CA-C	-6.43	106.39	114.56
1	F	240	PHE	CA-CB-CG	6.37	120.17	113.80
1	D	91	GLU	N-CA-C	-6.28	104.72	112.38
1	A	64	LEU	N-CA-C	-6.24	97.51	110.80
1	D	56	GLN	N-CA-C	-6.21	105.19	112.89
1	D	47	ALA	N-CA-C	-6.17	105.84	113.19
1	F	104	HIS	N-CA-C	-6.16	105.53	113.16
1	C	104	HIS	N-CA-C	-6.15	105.53	113.16
1	B	33	VAL	N-CA-C	-6.14	107.15	113.10
1	A	46	ALA	CA-C-O	-6.13	114.38	120.82
1	B	35	PHE	CA-CB-CG	6.11	119.91	113.80
1	A	339	LEU	CA-C-N	-6.10	113.26	121.80
1	A	339	LEU	C-N-CA	-6.10	113.26	121.80
1	E	92	ALA	N-CA-C	-6.06	103.24	111.55
1	E	86	THR	N-CA-C	-6.06	105.92	113.55
1	A	63	GLU	N-CA-C	-6.02	105.91	113.20
1	F	169	PHE	CA-CB-CG	5.99	119.79	113.80
1	A	91	GLU	N-CA-C	-5.99	105.69	112.87
1	E	102	MET	N-CA-C	-5.97	103.94	111.11
1	F	196	ASN	CB-CA-C	5.96	120.36	111.89
1	D	76	CYS	N-CA-C	-5.91	103.40	111.56
1	B	360	LYS	N-CA-C	-5.88	105.29	112.88
1	A	64	LEU	CA-C-N	-5.81	113.55	122.61
1	A	64	LEU	C-N-CA	-5.81	113.55	122.61
1	E	87	ILE	CA-C-O	-5.77	116.31	121.97
1	C	144	LYS	N-CA-C	-5.75	106.03	113.16
1	C	82	HIS	CB-CA-C	-5.75	101.82	110.90
1	F	225	PRO	N-CA-CB	-5.75	97.58	103.15
1	A	115	ALA	O-C-N	-5.72	116.14	122.09
1	F	31	GLU	CA-C-N	-5.70	115.75	123.10
1	F	31	GLU	C-N-CA	-5.70	115.75	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	CYS	O-C-N	-5.65	114.88	122.23
1	A	114	GLU	N-CA-C	-5.61	103.96	112.04
1	A	45	LYS	O-C-N	5.61	128.78	122.22
1	E	96	VAL	N-CA-C	5.55	116.12	108.12
1	E	94	LYS	N-CA-C	5.53	117.81	109.41
1	A	129	ASN	N-CA-C	-5.48	106.66	113.19
1	C	96	VAL	N-CA-C	5.48	115.78	108.11
1	D	50	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	112	MET	N-CA-C	-5.46	106.68	113.55
1	F	215	GLU	N-CA-CB	-5.41	101.88	110.22
1	D	57	VAL	CA-C-O	-5.39	114.04	120.78
1	F	235	ASP	N-CA-C	-5.36	106.91	113.50
1	A	131	PHE	CA-CB-CG	5.35	119.15	113.80
1	A	89	ALA	N-CA-C	-5.34	105.36	111.07
1	D	107	GLU	N-CA-CB	-5.31	102.30	110.16
1	A	43	ALA	CA-C-N	5.30	127.82	120.29
1	A	43	ALA	C-N-CA	5.30	127.82	120.29
1	D	360	LYS	N-CA-C	-5.30	106.66	113.02
1	F	85	ILE	N-CA-C	-5.29	98.34	109.34
1	E	38	ILE	N-CA-C	-5.27	104.50	111.09
1	E	270	CYS	O-C-N	5.26	129.56	123.30
1	F	117	LYS	N-CA-C	-5.25	105.25	110.97
1	E	123	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	62	LYS	CA-C-N	-5.19	111.56	121.94
1	A	62	LYS	C-N-CA	-5.19	111.56	121.94
1	C	97	TYR	CB-CA-C	-5.18	102.34	110.79
1	F	334	ASN	N-CA-C	-5.18	106.76	114.64
1	F	268	THR	CB-CA-C	5.17	119.06	109.70
1	A	76	CYS	N-CA-C	-5.17	104.27	110.88
1	F	78	PRO	CB-CA-C	5.16	119.35	111.40
1	D	14	ILE	N-CA-C	-5.12	105.55	110.72
1	F	190	ILE	N-CA-C	-5.11	105.41	110.62
1	F	41	ASP	CA-C-N	-5.09	112.69	121.66
1	F	41	ASP	C-N-CA	-5.09	112.69	121.66
1	B	127	TYR	CB-CA-C	5.06	119.56	112.07
1	A	46	ALA	N-CA-C	5.06	116.49	111.07
1	F	186	HIS	CA-CB-CG	5.06	118.86	113.80
1	D	37	ASP	CB-CA-C	5.05	118.72	110.03
1	E	104	HIS	CA-CB-CG	5.05	118.85	113.80
1	B	104	HIS	CA-C-N	5.04	130.16	122.65
1	B	104	HIS	C-N-CA	5.04	130.16	122.65
1	E	95	HIS	CA-CB-CG	5.03	118.83	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	235	ASP	CA-CB-CG	5.02	117.62	112.60

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	2574	0	2448	197	0
1	B	2687	0	2598	95	0
1	C	2674	0	2591	128	0
1	D	2639	0	2514	152	0
1	E	2679	0	2586	100	0
1	F	2621	0	2485	158	0
2	A	12	0	12	5	0
2	C	12	0	11	1	0
2	D	12	0	11	5	0
2	E	12	0	11	0	0
2	F	12	0	12	1	0
3	A	44	0	26	7	0
3	B	44	0	26	6	0
3	C	44	0	25	7	0
3	D	44	0	26	6	0
3	E	44	0	25	6	0
3	F	44	0	25	10	0
4	A	33	0	0	0	0
4	B	53	0	0	0	0
4	C	31	0	0	2	0
4	D	30	0	0	2	0
4	E	40	0	0	0	0
4	F	37	0	0	2	0
All	All	16422	0	15432	808	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 26.

All (808) 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:D:86:THR:C	1:D:88:ALA:N	2.01	1.18
1:F:6:ILE:HB	1:F:32:ILE:CD1	1.76	1.15
1:A:56:GLN:HE21	1:A:63:GLU:HB3	1.08	1.09
1:A:79:ASN:HD22	1:A:175:GLN:CD	1.64	1.06
1:A:100:LYS:HE2	1:A:186:HIS:NE2	1.71	1.05
1:A:44:GLU:O	1:A:57:VAL:HG11	1.56	1.03
1:A:56:GLN:NE2	1:A:63:GLU:HB3	1.71	1.03
1:D:40:ILE:HG23	1:D:59:ALA:HB2	1.38	1.02
1:F:6:ILE:CB	1:F:32:ILE:HD12	1.88	1.02
1:E:100:LYS:HB3	1:E:101:PRO:HD3	1.37	1.01
1:C:100:LYS:HD2	1:C:185:THR:HG21	1.42	0.97
1:F:35:PHE:CE2	1:F:47:ALA:HA	2.00	0.96
1:A:79:ASN:ND2	1:A:175:GLN:CD	2.24	0.96
1:B:84:GLU:O	1:B:88:ALA:HB2	1.66	0.96
1:D:52:ALA:HB1	1:D:55:ALA:HB2	1.44	0.95
1:F:6:ILE:HB	1:F:32:ILE:HD12	0.96	0.95
1:A:78:PRO:HG3	1:A:168:VAL:HG11	1.51	0.93
1:A:4:LEU:HD12	1:A:333:GLN:HG2	1.48	0.92
1:D:52:ALA:CB	1:D:55:ALA:HB2	1.98	0.92
1:D:9:ILE:HD13	1:D:61:TYR:HB2	1.52	0.91
1:A:61:TYR:HB2	3:A:402:NAD:N1A	1.86	0.91
1:C:86:THR:HG23	1:C:96:VAL:HG11	1.52	0.91
1:A:5:LYS:HA	1:A:31:GLU:HB3	1.51	0.90
1:A:44:GLU:O	1:A:57:VAL:CG1	2.20	0.89
1:B:282:MET:HE3	1:B:282:MET:HA	1.54	0.89
1:A:79:ASN:ND2	1:A:175:GLN:NE2	2.20	0.88
1:A:109:ALA:HA	1:A:112:MET:HE3	1.56	0.88
1:D:100:LYS:HB3	1:D:101:PRO:HD3	1.55	0.87
1:E:87:ILE:O	1:E:88:ALA:C	2.18	0.87
1:A:106:THR:HG23	1:A:350:LYS:HG2	1.56	0.85
1:A:86:THR:HG23	1:A:96:VAL:HG11	1.59	0.84
1:F:8:ILE:HD13	1:F:20:PHE:HE1	1.42	0.84
1:C:90:PHE:C	1:C:92:ALA:H	1.86	0.84
1:F:86:THR:HG23	1:F:96:VAL:HG21	1.58	0.84
1:A:75:VAL:HG22	1:A:98:CYS:HA	1.59	0.83
1:D:212:GLY:O	1:D:226:TRP:CZ3	2.31	0.83
1:D:26:ASN:OD1	1:D:326:ARG:HD2	1.78	0.83
1:C:100:LYS:HD2	1:C:185:THR:CG2	2.09	0.83
1:D:128:GLN:HE22	3:D:402:NAD:H72N	1.26	0.83
1:E:87:ILE:HD11	1:E:111:LYS:HB2	1.60	0.82
1:A:64:LEU:C	1:A:66:ALA:N	2.34	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:GLY:O	1:D:226:TRP:HZ3	1.63	0.81
1:E:88:ALA:O	1:E:89:ALA:C	2.23	0.81
1:F:65:LEU:HD13	1:F:89:ALA:O	1.81	0.80
1:D:56:GLN:OE1	1:D:64:LEU:HA	1.82	0.80
1:A:159:ARG:HD3	1:A:162:ALA:HB3	1.63	0.79
1:B:100:LYS:HD2	1:B:186:HIS:NE2	1.97	0.79
1:C:212:GLY:O	1:C:226:TRP:HZ3	1.65	0.79
1:A:62:LYS:HA	1:A:65:LEU:HD13	1.65	0.78
1:E:91:GLU:HG2	1:E:116:TRP:HA	1.64	0.77
1:F:122:GLN:HG3	1:F:332:ILE:HG22	1.64	0.77
1:F:8:ILE:HD13	1:F:20:PHE:CE1	2.18	0.77
1:F:100:LYS:HG3	1:F:101:PRO:HD3	1.67	0.77
1:C:357:LYS:HD2	1:C:364:ILE:HG12	1.66	0.76
1:F:86:THR:HA	1:F:90:PHE:CB	2.15	0.76
1:D:100:LYS:HE2	1:D:101:PRO:HG3	1.68	0.75
1:F:163:VAL:HG22	1:F:255:TRP:HB3	1.68	0.75
1:C:172:LYS:O	1:C:172:LYS:HD3	1.85	0.75
1:E:100:LYS:HB3	1:E:101:PRO:CD	2.15	0.75
1:A:60:ASP:OD1	1:A:63:GLU:HB2	1.87	0.75
1:C:164:PRO:O	1:C:170:MET:HE2	1.86	0.75
1:A:64:LEU:C	1:A:66:ALA:H	1.94	0.75
1:D:188:LEU:HG	1:D:251:LEU:HD12	1.69	0.75
1:E:212:GLY:O	1:E:226:TRP:HZ3	1.69	0.75
1:A:106:THR:CG2	1:A:350:LYS:HG2	2.16	0.74
1:A:102:MET:HE1	1:A:113:VAL:HG12	1.70	0.74
1:C:186:HIS:ND1	4:C:501:HOH:O	2.21	0.74
1:E:100:LYS:CB	1:E:101:PRO:HD3	2.17	0.74
1:A:359:ALA:C	1:A:361:THR:H	1.94	0.74
1:B:88:ALA:C	1:B:90:PHE:H	1.95	0.74
1:B:100:LYS:HG3	1:B:101:PRO:HD3	1.68	0.74
1:B:212:GLY:O	1:B:226:TRP:HZ3	1.70	0.74
1:D:129:ASN:OD1	1:D:132:ARG:NH1	2.20	0.74
1:C:168:VAL:HG13	3:C:402:NAD:O2A	1.86	0.73
1:E:161:ARG:HG2	1:E:221:ASN:HA	1.70	0.73
1:C:177:GLY:N	1:C:181:ILE:HD11	2.04	0.73
1:B:100:LYS:HE2	1:B:101:PRO:HG3	1.71	0.72
1:B:88:ALA:C	1:B:90:PHE:N	2.45	0.72
1:C:124:THR:O	1:C:125:ILE:HD13	1.88	0.72
1:C:128:GLN:HE22	3:C:402:NAD:H72N	1.35	0.72
1:F:201:ASP:CG	1:F:365:LYS:HE2	2.14	0.72
1:F:212:GLY:O	1:F:226:TRP:HZ3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:CG	1:A:63:GLU:H	1.97	0.72
1:A:60:ASP:OD2	1:A:63:GLU:N	2.23	0.72
1:A:79:ASN:HD21	1:A:175:GLN:NE2	1.88	0.72
1:F:40:ILE:HB	1:F:59:ALA:HB2	1.72	0.72
1:A:128:GLN:HE22	3:A:402:NAD:H72N	1.36	0.72
1:A:171:ASP:OD2	1:A:174:ALA:CB	2.36	0.72
1:E:87:ILE:O	1:E:89:ALA:N	2.22	0.72
1:E:82:HIS:CE1	3:E:402:NAD:O3D	2.43	0.72
1:C:188:LEU:O	1:C:188:LEU:HD23	1.90	0.72
1:F:88:ALA:HA	1:F:92:ALA:H	1.54	0.72
1:F:116:TRP:CD1	1:F:123:PHE:HB2	2.24	0.71
1:A:4:LEU:CD1	1:A:333:GLN:HG2	2.19	0.71
1:A:20:PHE:HB2	1:A:21:PRO:HD3	1.72	0.71
1:A:84:GLU:O	1:A:89:ALA:HB2	1.90	0.71
1:D:100:LYS:HE2	1:D:101:PRO:HD3	1.73	0.71
1:F:65:LEU:HD22	1:F:94:LYS:HE3	1.72	0.71
1:C:286:LYS:HD2	1:C:287:ASN:N	2.05	0.71
1:E:164:PRO:O	1:E:170:MET:HE2	1.89	0.71
1:B:212:GLY:O	1:B:226:TRP:CZ3	2.44	0.71
1:A:297:ASN:HA	1:F:219:GLU:HG2	1.74	0.70
1:A:44:GLU:O	1:A:57:VAL:CB	2.39	0.70
1:F:326:ARG:O	1:F:330:GLU:HG3	1.91	0.70
1:A:8:ILE:HG12	1:A:20:PHE:HE1	1.55	0.70
1:A:214:LYS:NZ	1:A:216:ASN:OD1	2.25	0.70
1:C:359:ALA:C	1:C:361:THR:H	1.99	0.70
1:F:106:THR:HG23	1:F:350:LYS:HG2	1.73	0.70
1:A:44:GLU:HA	1:A:57:VAL:HB	1.74	0.70
1:E:163:VAL:HG22	1:E:255:TRP:HB3	1.74	0.70
1:B:262:SER:HB2	1:B:283:SER:OG	1.92	0.69
1:B:319:GLU:OE1	1:B:319:GLU:HA	1.91	0.69
1:C:100:LYS:HD3	1:C:186:HIS:NE2	2.07	0.69
1:A:78:PRO:HD3	3:A:402:NAD:H51A	1.74	0.69
1:A:87:ILE:C	1:A:89:ALA:H	1.98	0.69
1:F:130:ARG:HA	1:F:135:VAL:HG11	1.73	0.69
1:B:128:GLN:HE22	3:B:401:NAD:H72N	1.41	0.69
1:B:357:LYS:C	1:B:359:ALA:H	2.00	0.69
1:D:33:VAL:O	1:D:35:PHE:N	2.25	0.69
1:D:139:LYS:HE3	1:D:143:ASP:OD2	1.92	0.69
1:A:84:GLU:C	1:A:86:THR:H	1.98	0.69
1:C:82:HIS:CE1	3:C:402:NAD:O3D	2.45	0.69
1:A:27:ALA:O	1:A:29:LEU:N	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ILE:HD12	1:B:73:VAL:HG13	1.74	0.69
1:F:100:LYS:HD3	1:F:186:HIS:NE2	2.08	0.69
1:A:219:GLU:HG3	1:F:297:ASN:HA	1.74	0.69
1:F:169:PHE:HA	1:F:175:GLN:HG3	1.75	0.69
1:B:60:ASP:HB3	1:B:63:GLU:HG2	1.74	0.68
1:B:89:ALA:HA	1:B:92:ALA:CB	2.23	0.68
1:A:159:ARG:NH2	2:A:401:BGC:H1	2.08	0.68
1:F:75:VAL:HG21	1:F:86:THR:OG1	1.93	0.68
1:A:4:LEU:HD12	1:A:333:GLN:CG	2.23	0.68
1:A:14:ILE:HG21	1:A:99:GLU:HG3	1.75	0.68
1:E:105:SER:OG	1:E:108:GLU:HB2	1.92	0.68
1:D:7:GLY:C	1:D:8:ILE:HD13	2.20	0.67
1:D:100:LYS:HE2	1:D:101:PRO:CG	2.25	0.67
1:F:33:VAL:HG21	1:F:70:VAL:HG12	1.75	0.67
1:E:90:PHE:C	1:E:92:ALA:H	2.01	0.67
1:A:67:ASN:O	1:A:70:VAL:HG23	1.94	0.67
1:F:83:SER:O	1:F:87:ILE:HG12	1.95	0.67
1:D:44:GLU:O	1:D:46:ALA:N	2.27	0.67
1:A:57:VAL:O	1:A:58:THR:O	2.12	0.67
1:A:95:HIS:ND1	1:A:121:LYS:HB3	2.09	0.67
1:D:45:LYS:O	1:D:49:GLU:HG3	1.95	0.67
1:E:100:LYS:O	1:E:101:PRO:C	2.38	0.67
1:A:75:VAL:CG2	1:A:98:CYS:HA	2.25	0.67
1:E:357:LYS:C	1:E:359:ALA:H	2.03	0.67
1:B:89:ALA:HA	1:B:92:ALA:HB3	1.76	0.66
1:E:77:THR:O	3:E:402:NAD:H4D	1.95	0.66
1:E:106:THR:CG2	1:E:350:LYS:HG3	2.25	0.66
1:A:58:THR:OG1	1:A:59:ALA:N	2.20	0.66
1:C:360:LYS:HZ1	1:C:364:ILE:HG13	1.61	0.66
1:A:56:GLN:OE1	1:A:56:GLN:N	2.21	0.66
1:A:4:LEU:O	1:A:31:GLU:N	2.28	0.65
1:C:165:THR:HA	1:C:170:MET:HE1	1.78	0.65
1:F:23:LEU:HD22	1:F:32:ILE:HD11	1.77	0.65
1:D:57:VAL:HG22	1:D:57:VAL:O	1.96	0.65
1:E:87:ILE:HD11	1:E:111:LYS:CB	2.25	0.65
1:D:100:LYS:HE2	1:D:101:PRO:CD	2.26	0.65
1:E:82:HIS:NE2	3:E:402:NAD:O3D	2.29	0.65
1:E:212:GLY:O	1:E:226:TRP:CZ3	2.49	0.65
1:D:100:LYS:HE3	1:D:182:ASP:O	1.97	0.65
1:A:268:THR:O	1:A:269:LEU:HD23	1.97	0.65
1:A:100:LYS:HE2	1:A:186:HIS:CE1	2.32	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:SER:O	1:A:121:LYS:N	2.25	0.64
1:D:11:CYS:O	1:D:16:ASN:ND2	2.30	0.64
1:A:84:GLU:C	1:A:86:THR:N	2.52	0.64
1:F:88:ALA:O	1:F:89:ALA:C	2.40	0.64
1:A:67:ASN:O	1:A:69:GLU:N	2.30	0.64
1:C:165:THR:HA	1:C:170:MET:CE	2.27	0.64
1:C:199:ASP:OD1	1:C:244:LYS:HG3	1.98	0.64
1:D:52:ALA:O	1:D:53:GLU:C	2.39	0.64
1:A:114:GLU:HG3	1:A:115:ALA:H	1.63	0.64
1:B:285:PRO:O	1:B:286:LYS:HD3	1.98	0.64
1:F:87:ILE:O	1:F:89:ALA:N	2.25	0.64
1:F:91:GLU:HG2	1:F:115:ALA:O	1.97	0.64
1:A:4:LEU:CD1	1:A:332:ILE:HG13	2.28	0.64
1:E:165:THR:HA	1:E:170:MET:CE	2.27	0.64
1:D:100:LYS:HD3	1:D:186:HIS:NE2	2.13	0.63
1:E:90:PHE:C	1:E:92:ALA:N	2.56	0.63
1:B:100:LYS:HE2	1:B:101:PRO:HD3	1.80	0.63
1:C:100:LYS:NZ	1:C:101:PRO:HG3	2.14	0.63
1:D:44:GLU:C	1:D:46:ALA:H	2.05	0.63
1:A:64:LEU:O	1:A:65:LEU:C	2.38	0.63
1:A:141:SER:HB3	1:D:295:ARG:HH21	1.63	0.63
1:D:357:LYS:C	1:D:359:ALA:H	2.05	0.63
1:E:165:THR:HA	1:E:170:MET:HE2	1.81	0.63
1:B:90:PHE:C	1:B:92:ALA:H	2.06	0.63
1:C:82:HIS:NE2	3:C:402:NAD:O3D	2.32	0.63
1:A:16:ASN:OD1	1:A:20:PHE:HD2	1.82	0.63
1:A:60:ASP:CG	1:A:61:TYR:N	2.56	0.63
1:C:31:GLU:OE1	1:C:52:ALA:HB1	1.98	0.63
1:D:161:ARG:NH2	1:D:258:ASN:OD1	2.32	0.63
1:F:117:LYS:C	1:F:119:SER:H	2.07	0.63
1:A:7:GLY:O	1:A:73:VAL:HA	1.99	0.63
1:A:14:ILE:O	1:A:19:HIS:HD2	1.82	0.63
1:A:87:ILE:O	1:A:89:ALA:N	2.26	0.63
1:C:159:ARG:HD3	1:C:162:ALA:HB3	1.81	0.63
1:B:328:TRP:CZ2	1:B:332:ILE:HD11	2.33	0.62
1:F:117:LYS:O	1:F:119:SER:N	2.30	0.62
1:B:42:ARG:NH2	3:B:401:NAD:O3B	2.31	0.62
1:D:169:PHE:HA	1:D:175:GLN:HG3	1.80	0.62
1:C:29:LEU:CD2	1:C:326:ARG:NH2	2.62	0.62
1:A:60:ASP:CG	1:A:63:GLU:HB2	2.24	0.62
1:E:15:ALA:HA	1:E:19:HIS:HB2	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:VAL:HG21	1:F:70:VAL:CG1	2.29	0.62
1:F:201:ASP:OD2	1:F:365:LYS:HE2	2.00	0.62
1:C:212:GLY:O	1:C:226:TRP:CZ3	2.52	0.62
1:E:5:LYS:HE3	1:E:69:GLU:O	1.99	0.61
1:F:40:ILE:HD11	1:F:57:VAL:HG12	1.82	0.61
1:C:33:VAL:HG23	1:C:55:ALA:HA	1.82	0.61
1:A:100:LYS:CE	1:A:186:HIS:NE2	2.58	0.61
1:F:40:ILE:HD11	1:F:57:VAL:O	2.01	0.61
1:B:100:LYS:HE2	1:B:101:PRO:CG	2.29	0.61
1:D:11:CYS:SG	1:D:36:CYS:O	2.56	0.61
1:A:68:PRO:C	1:A:70:VAL:H	2.05	0.61
1:F:79:ASN:HD21	1:F:101:PRO:HG2	1.65	0.61
1:A:88:ALA:H	1:A:91:GLU:CB	2.14	0.61
3:F:402:NAD:H6N	3:F:402:NAD:O1N	2.01	0.61
1:A:111:LYS:HA	1:A:114:GLU:HG2	1.83	0.61
1:C:33:VAL:HG23	1:C:56:GLN:H	1.65	0.61
1:D:158:VAL:HG11	1:D:259:MET:HE2	1.82	0.61
1:F:31:GLU:C	1:F:32:ILE:HD13	2.25	0.61
1:A:319:GLU:HA	1:A:319:GLU:OE1	2.00	0.61
1:D:44:GLU:C	1:D:46:ALA:N	2.58	0.61
1:E:102:MET:HE2	1:E:123:PHE:CE2	2.35	0.60
1:E:106:THR:HG23	1:E:350:LYS:HG3	1.83	0.60
1:E:327:GLN:OE1	1:E:339:LEU:N	2.26	0.60
1:A:180:LEU:HB3	1:A:356:TYR:OH	2.00	0.60
1:A:6:ILE:N	1:A:31:GLU:O	2.20	0.60
1:A:150:ILE:HG21	1:A:195:MET:HG2	1.84	0.60
1:A:26:ASN:O	1:A:27:ALA:C	2.44	0.60
1:A:64:LEU:O	1:A:66:ALA:N	2.34	0.60
1:B:98:CYS:O	1:B:125:ILE:HA	2.01	0.60
1:D:8:ILE:HG13	1:D:20:PHE:HE1	1.66	0.60
1:A:87:ILE:C	1:A:89:ALA:N	2.59	0.60
1:D:159:ARG:HD3	1:D:162:ALA:HB3	1.82	0.60
1:D:279:HIS:HB2	1:D:288:GLU:HB2	1.82	0.60
1:F:83:SER:O	1:F:87:ILE:HG23	2.01	0.60
1:A:61:TYR:CD1	1:A:61:TYR:C	2.80	0.60
1:F:357:LYS:C	1:F:359:ALA:H	2.10	0.60
1:B:8:ILE:HD12	1:B:32:ILE:HG21	1.83	0.60
1:D:28:ASP:OD2	1:D:29:LEU:CD1	2.50	0.60
1:B:131:PHE:CE1	1:B:339:LEU:HD23	2.37	0.60
1:F:88:ALA:O	1:F:92:ALA:N	2.35	0.60
1:E:128:GLN:HE22	3:E:402:NAD:H72N	1.48	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ALA:CA	1:B:92:ALA:HB3	2.33	0.59
1:B:106:THR:O	1:B:110:GLU:HG3	2.01	0.59
1:C:286:LYS:HD2	1:C:287:ASN:H	1.68	0.59
1:C:357:LYS:HG2	1:C:360:LYS:HE3	1.85	0.59
1:D:39:GLN:HB2	1:D:42:ARG:CB	2.31	0.59
1:B:205:GLY:HA3	1:B:355:ILE:HG23	1.83	0.59
1:C:297:ASN:HA	1:D:219:GLU:HG3	1.83	0.59
1:D:188:LEU:HG	1:D:251:LEU:CD1	2.33	0.59
1:A:60:ASP:OD2	1:A:62:LYS:N	2.36	0.59
1:E:107:GLU:O	1:E:111:LYS:HG3	2.02	0.59
1:F:74:HIS:CD2	1:F:97:TYR:HB3	2.38	0.59
1:A:171:ASP:OD2	1:A:174:ALA:HB3	2.03	0.59
1:F:128:GLN:HE22	3:F:402:NAD:H72N	1.49	0.59
1:D:234:GLU:OE1	1:D:234:GLU:N	2.30	0.58
1:E:88:ALA:O	1:E:90:PHE:N	2.36	0.58
1:F:35:PHE:CD2	1:F:47:ALA:HB2	2.38	0.58
1:F:216:ASN:O	1:F:219:GLU:HB2	2.03	0.58
1:E:214:LYS:HE3	1:E:216:ASN:OD1	2.03	0.58
1:B:212:GLY:HA2	1:B:226:TRP:CH2	2.38	0.58
1:E:159:ARG:HD3	1:E:162:ALA:HB3	1.85	0.58
1:F:88:ALA:CA	1:F:92:ALA:H	2.15	0.58
1:A:13:GLY:O	1:A:17:GLN:N	2.31	0.58
1:B:90:PHE:C	1:B:92:ALA:N	2.61	0.58
1:C:32:ILE:CG2	1:C:35:PHE:CZ	2.87	0.58
1:A:157:ALA:O	1:A:253:ALA:HA	2.04	0.58
1:B:183:ILE:HD11	1:B:254:SER:O	2.04	0.58
1:C:102:MET:HE2	1:C:123:PHE:CE2	2.39	0.58
1:C:108:GLU:O	1:C:112:MET:HG3	2.04	0.58
1:A:67:ASN:N	1:A:68:PRO:HD3	2.19	0.58
1:B:89:ALA:O	1:B:92:ALA:HB3	2.03	0.58
1:D:109:ALA:O	1:D:113:VAL:HG23	2.03	0.58
1:A:67:ASN:C	1:A:69:GLU:N	2.61	0.58
1:D:205:GLY:HA3	1:D:355:ILE:HG23	1.86	0.58
1:D:79:ASN:HD22	1:D:82:HIS:CE1	2.21	0.57
1:F:8:ILE:HD12	1:F:32:ILE:HG21	1.86	0.57
1:F:127:TYR:OH	1:F:185:THR:OG1	2.21	0.57
1:C:100:LYS:CD	1:C:185:THR:HG21	2.25	0.57
1:F:179:PRO:HD3	1:F:255:TRP:CE3	2.39	0.57
1:A:68:PRO:C	1:A:70:VAL:N	2.62	0.57
1:A:47:ALA:H	1:A:57:VAL:HG12	1.68	0.57
1:D:188:LEU:HD12	1:D:352:LEU:HD21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ALA:HB1	1:D:55:ALA:CB	2.27	0.57
1:C:49:GLU:HB2	1:C:50:PHE:CD1	2.40	0.57
1:D:195:MET:HE1	1:D:249:ILE:HD11	1.87	0.57
1:B:100:LYS:HE2	1:B:101:PRO:CD	2.35	0.57
1:F:60:ASP:O	1:F:63:GLU:HB2	2.05	0.57
1:F:95:HIS:CE1	1:F:121:LYS:HD3	2.39	0.57
1:C:294:ALA:HB1	1:D:219:GLU:HG2	1.87	0.57
1:D:95:HIS:CE1	1:D:121:LYS:HD3	2.39	0.57
1:F:3:LYS:HE3	1:F:27:ALA:O	2.05	0.57
1:B:159:ARG:HD3	1:B:162:ALA:HB3	1.85	0.56
1:F:93:GLY:C	1:F:94:LYS:HG3	2.30	0.56
1:F:164:PRO:HB2	1:F:169:PHE:CD2	2.39	0.56
1:A:325:ASN:HD21	1:A:329:LEU:HD11	1.70	0.56
1:A:359:ALA:C	1:A:361:THR:N	2.61	0.56
1:B:222:LEU:HD23	1:B:223:PHE:CZ	2.39	0.56
1:C:25:ASN:HD22	1:C:322:THR:HG21	1.69	0.56
1:F:87:ILE:C	1:F:89:ALA:N	2.63	0.56
1:A:168:VAL:HG13	3:A:402:NAD:O2A	2.05	0.56
1:B:266:SER:HB3	1:B:278:ILE:O	2.06	0.56
1:C:172:LYS:HB2	1:C:232:GLU:HG3	1.88	0.56
1:D:75:VAL:HB	1:D:98:CYS:HA	1.87	0.56
1:A:47:ALA:H	1:A:57:VAL:CG1	2.19	0.56
1:D:154:LYS:HB2	1:D:268:THR:HB	1.87	0.56
1:F:100:LYS:HA	1:F:125:ILE:HG22	1.87	0.56
1:F:160:ARG:O	1:F:256:ALA:HA	2.04	0.56
1:A:159:ARG:HH22	2:A:401:BGC:H1	1.70	0.56
1:C:154:LYS:HE3	1:D:252:GLU:OE2	2.06	0.56
1:D:50:PHE:O	1:D:52:ALA:N	2.39	0.56
1:B:303:THR:HG22	1:F:301:GLU:HG3	1.88	0.56
1:F:222:LEU:O	1:F:223:PHE:HB2	2.06	0.56
1:D:46:ALA:C	1:D:48:ALA:H	2.11	0.56
1:D:266:SER:HB3	1:D:278:ILE:O	2.06	0.56
1:E:89:ALA:O	1:E:90:PHE:CB	2.53	0.56
1:A:44:GLU:O	1:A:57:VAL:HB	2.06	0.55
1:A:56:GLN:HG2	1:A:58:THR:HG22	1.88	0.55
1:D:46:ALA:C	1:D:48:ALA:N	2.63	0.55
1:C:188:LEU:HD23	1:C:188:LEU:C	2.31	0.55
1:D:79:ASN:ND2	3:D:402:NAD:O3D	2.39	0.55
1:F:79:ASN:ND2	1:F:101:PRO:HG2	2.21	0.55
1:A:150:ILE:CG2	1:A:195:MET:HG2	2.37	0.55
1:A:279:HIS:HB2	1:A:288:GLU:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:GLY:HA3	1:E:355:ILE:HG23	1.88	0.55
1:F:4:LEU:CD1	1:F:332:ILE:HG13	2.36	0.55
1:F:99:GLU:HG3	3:F:402:NAD:H1D	1.88	0.55
1:A:78:PRO:CG	1:A:168:VAL:HG11	2.31	0.55
1:A:114:GLU:HG3	1:A:115:ALA:N	2.22	0.55
1:B:8:ILE:HD13	1:B:20:PHE:HE1	1.71	0.55
1:C:32:ILE:HG22	1:C:35:PHE:CE1	2.41	0.55
1:A:75:VAL:HG23	1:A:75:VAL:O	2.05	0.55
1:B:88:ALA:O	1:B:90:PHE:N	2.39	0.55
1:C:251:LEU:HD23	1:C:252:GLU:N	2.22	0.55
1:A:179:PRO:HA	1:A:182:ASP:HB3	1.88	0.55
1:C:277:GLU:OE1	1:C:279:HIS:NE2	2.32	0.55
1:C:172:LYS:HD3	1:C:172:LYS:C	2.32	0.55
1:D:28:ASP:OD2	1:D:29:LEU:HD12	2.05	0.55
1:D:100:LYS:CB	1:D:101:PRO:HD3	2.34	0.55
1:E:158:VAL:HG11	1:E:259:MET:HE2	1.88	0.55
1:F:30:ASN:HD22	1:F:329:LEU:CD1	2.19	0.55
1:A:4:LEU:HD13	1:A:332:ILE:CD1	2.37	0.55
1:A:67:ASN:C	1:A:69:GLU:H	2.15	0.55
1:C:357:LYS:O	1:C:360:LYS:HG2	2.07	0.54
1:E:79:ASN:ND2	3:E:402:NAD:O3D	2.40	0.54
1:A:86:THR:HG22	1:A:87:ILE:H	1.72	0.54
1:A:110:GLU:HG3	1:A:346:LEU:HD11	1.88	0.54
1:A:169:PHE:CE1	2:A:401:BGC:H3	2.43	0.54
1:C:12:GLY:HA3	3:C:402:NAD:O5B	2.07	0.54
1:C:359:ALA:C	1:C:361:THR:N	2.65	0.54
1:F:106:THR:CG2	1:F:350:LYS:HG2	2.38	0.54
1:D:159:ARG:HH12	2:D:401:BGC:C6	2.21	0.54
1:F:86:THR:O	1:F:91:GLU:OE1	2.25	0.54
1:C:185:THR:HG23	1:C:186:HIS:N	2.22	0.54
1:D:89:ALA:O	1:D:92:ALA:HB3	2.08	0.54
1:B:95:HIS:CE1	1:B:121:LYS:HD2	2.43	0.54
1:B:157:ALA:O	1:B:253:ALA:HA	2.07	0.54
1:B:202:SER:HB3	1:B:365:LYS:HD3	1.89	0.54
1:D:164:PRO:HG3	2:D:401:BGC:O6	2.07	0.54
1:F:35:PHE:CD2	1:F:47:ALA:HA	2.41	0.53
1:B:108:GLU:O	1:B:112:MET:HG3	2.08	0.53
1:E:136:MET:HE1	1:E:339:LEU:CD2	2.39	0.53
1:F:6:ILE:CB	1:F:32:ILE:CD1	2.66	0.53
1:F:201:ASP:O	1:F:365:LYS:HD2	2.08	0.53
1:F:35:PHE:CD2	1:F:47:ALA:CB	2.92	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:HG23	1:B:96:VAL:HG11	1.89	0.53
1:C:32:ILE:HG21	1:C:35:PHE:CZ	2.44	0.53
1:A:114:GLU:O	1:A:115:ALA:C	2.45	0.53
1:B:8:ILE:HD12	1:B:32:ILE:CG2	2.39	0.53
1:C:49:GLU:HB2	1:C:50:PHE:CE1	2.44	0.53
1:D:128:GLN:NE2	3:D:402:NAD:H72N	2.02	0.53
1:B:226:TRP:CZ3	1:B:231:PHE:CD2	2.97	0.53
1:C:198:TYR:CZ	1:C:344:GLU:HG2	2.44	0.52
1:D:100:LYS:HZ3	3:D:402:NAD:C2N	2.22	0.52
1:E:106:THR:HG21	1:E:350:LYS:HG3	1.91	0.52
1:F:95:HIS:ND1	1:F:121:LYS:HD3	2.23	0.52
1:B:20:PHE:HB2	1:B:21:PRO:HD3	1.90	0.52
1:C:266:SER:HB3	1:C:278:ILE:O	2.09	0.52
1:D:277:GLU:OE1	1:D:279:HIS:NE2	2.29	0.52
1:F:87:ILE:C	1:F:89:ALA:H	2.17	0.52
1:D:14:ILE:HG21	1:D:99:GLU:HG3	1.90	0.52
1:B:279:HIS:HB3	1:B:284:TYR:CE1	2.45	0.52
1:A:79:ASN:ND2	1:A:175:GLN:OE1	2.35	0.52
1:C:196:ASN:ND2	4:C:506:HOH:O	2.43	0.52
1:D:157:ALA:O	1:D:253:ALA:HA	2.09	0.52
1:E:266:SER:HB3	1:E:278:ILE:O	2.09	0.52
2:F:401:BGC:H3	3:F:402:NAD:C4N	2.39	0.52
1:A:4:LEU:HD13	1:A:332:ILE:HG13	1.92	0.52
1:A:90:PHE:C	1:A:92:ALA:N	2.67	0.52
1:D:7:GLY:O	1:D:8:ILE:HD13	2.10	0.52
1:F:79:ASN:ND2	3:F:402:NAD:O3D	2.43	0.52
1:C:122:GLN:NE2	1:C:336:THR:O	2.43	0.51
1:D:20:PHE:HB3	1:D:50:PHE:CZ	2.44	0.51
1:B:180:LEU:HD23	1:B:356:TYR:CE2	2.45	0.51
1:C:361:THR:O	1:C:361:THR:HG23	2.10	0.51
1:B:89:ALA:C	1:B:92:ALA:HB3	2.35	0.51
1:A:61:TYR:CB	3:A:402:NAD:N1A	2.69	0.51
1:A:79:ASN:OD1	1:A:101:PRO:HG2	2.11	0.51
1:C:354:ALA:O	1:C:364:ILE:HD13	2.10	0.51
1:B:357:LYS:C	1:B:359:ALA:N	2.66	0.51
1:C:157:ALA:O	1:C:253:ALA:HA	2.11	0.51
1:B:100:LYS:HD3	3:B:401:NAD:C2N	2.41	0.51
1:F:33:VAL:O	1:F:35:PHE:N	2.44	0.51
1:F:327:GLN:OE1	1:F:338:PRO:HA	2.11	0.51
1:F:20:PHE:HB2	1:F:21:PRO:HD3	1.93	0.51
1:F:100:LYS:CG	1:F:101:PRO:HD3	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ALA:O	1:D:50:PHE:HB2	2.10	0.51
1:A:329:LEU:O	1:A:332:ILE:HG12	2.11	0.50
1:C:28:ASP:CG	1:C:29:LEU:HD22	2.36	0.50
1:C:290:ILE:HG21	1:D:260:LEU:HD22	1.93	0.50
1:D:131:PHE:CZ	1:D:339:LEU:HD23	2.46	0.50
1:F:117:LYS:C	1:F:119:SER:N	2.67	0.50
1:F:212:GLY:HA2	1:F:226:TRP:CH2	2.47	0.50
1:A:27:ALA:C	1:A:29:LEU:H	2.19	0.50
1:B:222:LEU:HD23	1:B:223:PHE:CE1	2.46	0.50
1:D:52:ALA:HB3	1:D:55:ALA:HB2	1.87	0.50
1:D:90:PHE:C	1:D:92:ALA:N	2.67	0.50
1:D:122:GLN:HB2	1:D:332:ILE:CD1	2.41	0.50
1:E:364:ILE:HG22	1:E:366:PHE:CE1	2.47	0.50
1:A:325:ASN:O	1:A:328:TRP:HB3	2.11	0.50
1:D:131:PHE:CE1	1:D:339:LEU:HD22	2.47	0.50
1:A:8:ILE:HG12	1:A:20:PHE:CE1	2.42	0.50
1:B:41:ASP:OD1	1:B:42:ARG:N	2.45	0.50
1:E:8:ILE:HD13	1:E:74:HIS:HB2	1.92	0.50
1:F:99:GLU:OE2	3:F:402:NAD:H2N	2.11	0.50
1:F:153:GLY:O	1:F:249:ILE:HA	2.12	0.50
1:A:67:ASN:N	1:A:68:PRO:CD	2.74	0.50
1:A:268:THR:C	1:A:269:LEU:HD23	2.37	0.50
1:C:188:LEU:HD23	1:C:192:LEU:HG	1.94	0.50
1:D:104:HIS:ND1	1:D:104:HIS:N	2.59	0.50
1:D:217:GLY:N	1:D:218:PRO:CD	2.75	0.50
1:D:357:LYS:C	1:D:359:ALA:N	2.70	0.50
1:A:171:ASP:OD2	1:A:174:ALA:HB2	2.11	0.50
1:A:154:LYS:O	1:A:267:THR:HA	2.12	0.49
1:B:130:ARG:HD3	1:B:193:TRP:CE2	2.47	0.49
1:C:114:GLU:O	1:C:118:LYS:HG3	2.12	0.49
1:A:171:ASP:OD2	1:A:174:ALA:N	2.39	0.49
1:B:79:ASN:OD1	1:B:101:PRO:HG2	2.12	0.49
1:C:219:GLU:HG2	1:D:297:ASN:HA	1.93	0.49
2:D:401:BGC:H3	3:D:402:NAD:C5N	2.42	0.49
1:F:4:LEU:O	1:F:30:ASN:HA	2.11	0.49
1:C:29:LEU:HD23	1:C:326:ARG:NH2	2.27	0.49
1:A:56:GLN:NE2	1:A:63:GLU:O	2.36	0.49
1:C:161:ARG:HG2	1:C:221:ASN:HA	1.93	0.49
1:A:353:ASP:O	1:A:357:LYS:HD3	2.12	0.49
1:B:60:ASP:OD2	1:B:63:GLU:OE1	2.31	0.49
1:D:106:THR:CG2	1:D:350:LYS:HA	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LYS:HZ2	1:C:101:PRO:HG3	1.75	0.49
1:C:280:SER:HB2	1:C:287:ASN:OD1	2.13	0.49
1:D:106:THR:HG22	1:D:350:LYS:HA	1.94	0.49
1:D:188:LEU:HD12	1:D:352:LEU:CD2	2.41	0.49
1:C:93:GLY:O	1:C:121:LYS:HE2	2.13	0.49
1:D:15:ALA:HA	1:D:19:HIS:HB2	1.93	0.49
1:F:87:ILE:O	1:F:87:ILE:HG13	2.13	0.49
1:A:158:VAL:HG11	1:A:259:MET:HE2	1.94	0.49
1:D:213:GLN:HG2	1:D:228:PRO:O	2.13	0.49
1:A:63:GLU:C	1:A:64:LEU:O	2.53	0.49
1:E:163:VAL:CG2	1:E:255:TRP:HB3	2.42	0.49
1:F:12:GLY:HA3	3:F:402:NAD:O5B	2.13	0.49
1:B:100:LYS:HE3	1:B:182:ASP:O	2.12	0.48
1:B:154:LYS:HB2	1:B:268:THR:HB	1.94	0.48
1:C:1:MET:HE1	1:C:333:GLN:O	2.12	0.48
1:C:90:PHE:C	1:C:92:ALA:N	2.53	0.48
1:C:101:PRO:O	1:C:102:MET:C	2.55	0.48
1:A:23:LEU:O	1:A:27:ALA:N	2.46	0.48
1:A:273:GLU:OE1	1:F:214:LYS:NZ	2.43	0.48
1:E:29:LEU:HD23	1:E:333:GLN:OE1	2.13	0.48
1:E:277:GLU:OE1	1:E:279:HIS:NE2	2.29	0.48
1:F:24:LYS:O	1:F:27:ALA:N	2.47	0.48
1:C:188:LEU:C	1:C:188:LEU:CD2	2.86	0.48
1:E:279:HIS:HB2	1:E:288:GLU:HB2	1.95	0.48
1:F:217:GLY:C	1:F:219:GLU:H	2.20	0.48
1:A:55:ALA:HB1	1:A:56:GLN:OE1	2.13	0.48
1:A:202:SER:HB3	1:A:365:LYS:HE2	1.94	0.48
1:E:4:LEU:HD11	1:E:332:ILE:CG2	2.43	0.48
1:E:357:LYS:C	1:E:359:ALA:N	2.67	0.48
1:F:222:LEU:C	1:F:224:GLY:H	2.21	0.48
1:F:327:GLN:OE1	1:F:339:LEU:N	2.46	0.48
1:A:65:LEU:HD12	1:A:65:LEU:N	2.28	0.48
1:D:86:THR:HG23	1:D:96:VAL:HG11	1.94	0.48
1:F:221:ASN:C	1:F:222:LEU:O	2.55	0.48
1:A:77:THR:HB	1:A:81:SER:HB2	1.95	0.48
1:A:79:ASN:OD1	1:A:101:PRO:HB2	2.14	0.48
1:C:157:ALA:HA	1:C:264:GLU:HA	1.96	0.48
1:A:14:ILE:HG13	1:A:18:LYS:HD3	1.96	0.48
1:D:28:ASP:OD2	1:D:29:LEU:HD11	2.14	0.47
1:E:33:VAL:HG23	1:E:70:VAL:HG12	1.95	0.47
1:B:330:GLU:O	1:B:334:ASN:ND2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:ASN:ND2	1:F:222:LEU:O	2.47	0.47
1:A:56:GLN:HE22	1:A:63:GLU:C	2.20	0.47
1:A:61:TYR:CD1	1:A:61:TYR:O	2.66	0.47
1:B:85:ILE:O	1:B:90:PHE:CB	2.62	0.47
1:B:89:ALA:HA	1:B:92:ALA:HB2	1.95	0.47
1:D:212:GLY:O	1:D:226:TRP:CH2	2.67	0.47
1:A:91:GLU:C	1:A:93:GLY:N	2.69	0.47
1:C:188:LEU:CD2	1:C:192:LEU:HG	2.44	0.47
1:F:88:ALA:C	1:F:92:ALA:H	2.23	0.47
1:A:163:VAL:HG22	1:A:255:TRP:HB3	1.95	0.47
1:E:80:VAL:HA	1:E:104:HIS:CE1	2.50	0.47
1:D:116:TRP:CD1	1:D:123:PHE:HB2	2.49	0.47
1:E:100:LYS:CB	1:E:101:PRO:CD	2.85	0.47
1:A:99:GLU:OE2	1:A:100:LYS:N	2.47	0.47
1:B:163:VAL:HG22	1:B:255:TRP:HB3	1.96	0.47
1:D:29:LEU:CD1	1:D:326:ARG:NH1	2.78	0.47
1:D:100:LYS:HD2	1:D:185:THR:CG2	2.44	0.47
1:E:64:LEU:HD23	1:E:64:LEU:C	2.39	0.47
1:E:82:HIS:HE2	3:E:402:NAD:HO3N	1.62	0.47
1:E:161:ARG:HG2	1:E:221:ASN:CA	2.39	0.47
1:E:198:TYR:CZ	1:E:344:GLU:HG2	2.50	0.47
1:F:35:PHE:HE2	1:F:51:GLY:HA2	1.80	0.47
1:A:61:TYR:HA	3:A:402:NAD:H2A	1.96	0.47
1:D:129:ASN:HB3	1:D:190:ILE:HD11	1.97	0.47
1:B:226:TRP:CE3	1:B:231:PHE:HD2	2.33	0.47
1:E:78:PRO:HB3	1:E:174:ALA:HB1	1.96	0.47
1:C:222:LEU:HD23	1:C:282:MET:HE3	1.95	0.47
1:C:302:GLU:HA	1:E:301:GLU:O	2.14	0.47
1:D:29:LEU:HD12	1:D:29:LEU:N	2.30	0.47
1:D:38:ILE:H	1:D:38:ILE:HG13	1.50	0.47
1:D:262:SER:O	1:D:283:SER:HB2	2.15	0.47
1:F:84:GLU:C	1:F:85:ILE:O	2.54	0.47
1:A:27:ALA:C	1:A:29:LEU:N	2.73	0.46
1:C:212:GLY:HA2	1:C:226:TRP:CH2	2.50	0.46
1:D:79:ASN:HD21	1:D:101:PRO:HG2	1.80	0.46
1:D:118:LYS:HE2	1:D:118:LYS:HB2	1.60	0.46
1:C:252:GLU:OE1	1:D:152:TYR:OH	2.33	0.46
1:D:64:LEU:C	1:D:64:LEU:HD23	2.40	0.46
1:C:99:GLU:OE1	3:C:402:NAD:H2N	2.15	0.46
1:F:6:ILE:HG13	1:F:23:LEU:CD2	2.46	0.46
1:F:88:ALA:H	1:F:91:GLU:HB2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ALA:O	1:C:53:GLU:HB3	2.16	0.46
1:F:179:PRO:HD3	1:F:255:TRP:CD2	2.51	0.46
1:A:168:VAL:CG1	3:A:402:NAD:O2A	2.63	0.46
1:B:100:LYS:CG	3:B:401:NAD:H2N	2.45	0.46
1:C:28:ASP:N	1:C:28:ASP:OD1	2.49	0.46
1:C:168:VAL:CG1	3:C:402:NAD:O2A	2.61	0.46
1:F:36:CYS:HA	1:F:58:THR:O	2.16	0.46
1:C:238:VAL:HG12	1:D:240:PHE:HE1	1.80	0.46
1:D:236:SER:HB3	1:D:254:SER:OG	2.15	0.46
1:E:29:LEU:HD11	1:E:326:ARG:NH1	2.31	0.46
1:F:88:ALA:HA	1:F:92:ALA:N	2.26	0.46
1:A:150:ILE:HG22	1:A:195:MET:HE3	1.98	0.46
1:A:181:ILE:HG23	1:A:356:TYR:HE2	1.81	0.46
1:C:106:THR:CG2	1:C:350:LYS:HG2	2.46	0.46
1:E:83:SER:O	1:E:87:ILE:N	2.26	0.46
1:E:154:LYS:HB2	1:E:268:THR:HB	1.98	0.46
1:F:4:LEU:HD11	1:F:333:GLN:HG3	1.98	0.46
1:C:299:LEU:HD13	1:D:160:ARG:CD	2.45	0.46
1:D:35:PHE:CZ	1:D:50:PHE:HB2	2.51	0.46
1:E:100:LYS:HD3	1:E:185:THR:OG1	2.15	0.46
1:F:303:THR:HG22	1:F:304:LEU:N	2.31	0.46
1:A:33:VAL:O	1:A:33:VAL:HG22	2.15	0.46
1:A:175:GLN:OE1	1:A:175:GLN:HA	2.16	0.46
1:C:299:LEU:HD13	1:D:160:ARG:HD3	1.98	0.46
1:B:130:ARG:HD3	1:B:193:TRP:CD2	2.50	0.45
1:B:160:ARG:HD3	1:E:299:LEU:HD13	1.97	0.45
1:C:100:LYS:HB3	1:C:101:PRO:HD3	1.97	0.45
1:E:163:VAL:HG22	1:E:255:TRP:CB	2.45	0.45
1:A:64:LEU:O	1:A:65:LEU:HB2	2.16	0.45
1:C:100:LYS:HD3	1:C:186:HIS:CE1	2.50	0.45
1:E:268:THR:O	1:E:269:LEU:HD23	2.16	0.45
1:B:179:PRO:HB3	1:B:255:TRP:CD1	2.51	0.45
1:C:4:LEU:HD11	1:C:333:GLN:HG3	1.98	0.45
1:F:3:LYS:HB2	1:F:3:LYS:NZ	2.31	0.45
1:F:169:PHE:HZ	3:F:402:NAD:O1N	2.00	0.45
1:F:201:ASP:HB2	1:F:244:LYS:HG2	1.98	0.45
1:F:214:LYS:HB3	1:F:214:LYS:HE3	1.47	0.45
1:A:86:THR:HG22	1:A:87:ILE:N	2.31	0.45
1:D:35:PHE:HZ	1:D:50:PHE:HB2	1.81	0.45
1:F:40:ILE:HD13	1:F:59:ALA:N	2.31	0.45
1:A:103:SER:HB2	1:A:112:MET:HE1	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:THR:HB	1:C:78:PRO:CD	2.47	0.45
1:D:91:GLU:OE1	1:D:91:GLU:HA	2.16	0.45
1:D:159:ARG:NH1	2:D:401:BGC:O6	2.45	0.45
1:F:11:CYS:HA	1:F:15:ALA:CB	2.47	0.45
1:F:65:LEU:HD13	1:F:89:ALA:C	2.40	0.45
1:F:357:LYS:C	1:F:359:ALA:N	2.73	0.45
1:A:90:PHE:C	1:A:92:ALA:H	2.23	0.45
1:B:100:LYS:CE	1:B:101:PRO:HG3	2.43	0.45
1:B:226:TRP:CZ3	1:B:231:PHE:HD2	2.35	0.45
1:F:88:ALA:O	1:F:92:ALA:HB3	2.16	0.45
1:F:93:GLY:HA3	1:F:94:LYS:HE2	1.99	0.45
1:F:99:GLU:HG3	3:F:402:NAD:C1D	2.46	0.45
1:A:157:ALA:HA	1:A:264:GLU:HA	1.98	0.45
1:B:63:GLU:OE2	1:B:63:GLU:HA	2.16	0.45
1:C:148:GLY:HA3	1:C:273:GLU:HG2	1.97	0.45
1:C:205:GLY:HA3	1:C:355:ILE:HG23	1.99	0.45
1:C:222:LEU:CD2	1:C:282:MET:HE3	2.47	0.45
1:E:364:ILE:HD12	1:E:364:ILE:N	2.31	0.45
1:F:14:ILE:CG2	1:F:76:CYS:HB3	2.47	0.45
1:D:180:LEU:HD23	1:D:356:TYR:CE2	2.52	0.45
1:F:330:GLU:O	1:F:334:ASN:HB2	2.17	0.45
1:C:131:PHE:CE1	1:C:339:LEU:HD23	2.52	0.45
1:C:299:LEU:HD13	1:D:160:ARG:NE	2.32	0.45
1:D:150:ILE:HG21	1:D:195:MET:HG2	1.99	0.45
1:F:83:SER:O	1:F:87:ILE:CG2	2.65	0.45
1:A:14:ILE:CG2	1:A:99:GLU:HG3	2.45	0.44
1:A:359:ALA:O	1:A:361:THR:N	2.50	0.44
1:F:91:GLU:HG2	1:F:115:ALA:C	2.42	0.44
1:F:258:ASN:HB2	4:F:512:HOH:O	2.17	0.44
1:B:86:THR:C	1:B:88:ALA:H	2.24	0.44
1:D:357:LYS:O	1:D:359:ALA:N	2.49	0.44
1:E:139:LYS:HG2	1:E:193:TRP:CH2	2.53	0.44
1:A:358:SER:O	1:A:361:THR:N	2.50	0.44
1:D:8:ILE:HG13	1:D:20:PHE:CE1	2.49	0.44
1:A:75:VAL:CG2	1:A:75:VAL:O	2.65	0.44
1:A:161:ARG:NH2	1:A:258:ASN:OD1	2.50	0.44
1:B:131:PHE:CZ	1:B:339:LEU:HD23	2.52	0.44
1:F:35:PHE:CE2	1:F:51:GLY:HA2	2.51	0.44
1:A:7:GLY:O	1:A:74:HIS:N	2.40	0.44
1:A:159:ARG:NH2	1:A:183:ILE:HG21	2.33	0.44
1:B:65:LEU:HD22	1:B:90:PHE:HA	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:LEU:CD2	1:C:326:ARG:HH22	2.30	0.44
1:D:291:TYR:HB2	1:D:302:GLU:HB3	2.00	0.44
1:E:86:THR:HG23	1:E:96:VAL:HG11	1.99	0.44
1:F:52:ALA:O	1:F:53:GLU:CD	2.61	0.44
1:F:212:GLY:O	1:F:226:TRP:CZ3	2.60	0.44
1:A:354:ALA:HA	1:A:357:LYS:HB2	2.00	0.44
1:E:88:ALA:O	1:E:91:GLU:N	2.50	0.44
1:D:320:GLU:HG2	1:D:321:GLY:N	2.32	0.44
1:E:327:GLN:HE21	1:E:327:GLN:HB3	1.61	0.44
1:A:112:MET:C	1:A:114:GLU:N	2.70	0.44
1:B:100:LYS:HG2	3:B:401:NAD:H2N	2.00	0.44
1:C:286:LYS:HE3	1:C:287:ASN:O	2.18	0.44
1:C:320:GLU:HG2	1:C:321:GLY:N	2.32	0.44
1:D:100:LYS:HG2	1:D:185:THR:HG21	2.00	0.44
1:E:165:THR:HA	1:E:170:MET:HE1	1.98	0.44
1:F:37:ASP:HA	3:F:402:NAD:N3A	2.32	0.44
1:F:40:ILE:HD13	1:F:58:THR:C	2.43	0.44
1:F:129:ASN:HD22	1:F:129:ASN:H	1.66	0.44
1:A:61:TYR:O	1:A:61:TYR:HD1	2.00	0.44
1:A:159:ARG:HB2	1:A:255:TRP:HA	2.00	0.44
1:B:100:LYS:CG	1:B:101:PRO:HD3	2.43	0.44
1:C:1:MET:HE2	1:C:1:MET:HB3	1.78	0.44
1:A:44:GLU:CA	1:A:57:VAL:HB	2.44	0.43
1:A:86:THR:CG2	1:A:96:VAL:HG11	2.38	0.43
1:B:275:GLY:HA3	1:E:258:ASN:O	2.18	0.43
1:B:279:HIS:HB2	1:B:288:GLU:HB2	1.99	0.43
1:B:357:LYS:O	1:B:359:ALA:N	2.49	0.43
1:C:100:LYS:CB	1:C:101:PRO:HD3	2.48	0.43
1:E:337:GLU:CD	1:E:341:LYS:HE2	2.43	0.43
1:F:180:LEU:HD21	1:F:355:ILE:HB	1.98	0.43
1:A:114:GLU:CG	1:A:115:ALA:N	2.81	0.43
1:A:182:ASP:OD1	2:A:401:BGC:O4	2.35	0.43
1:D:80:VAL:HG13	1:D:81:SER:N	2.33	0.43
1:F:33:VAL:O	1:F:33:VAL:HG23	2.17	0.43
1:F:214:LYS:NZ	1:F:216:ASN:OD1	2.41	0.43
1:C:60:ASP:OD1	1:C:60:ASP:C	2.61	0.43
1:C:166:TRP:CD1	1:C:167:GLY:N	2.87	0.43
1:C:290:ILE:HG21	1:D:260:LEU:CD2	2.48	0.43
1:E:103:SER:OG	1:E:104:HIS:N	2.49	0.43
1:E:106:THR:HG23	1:E:350:LYS:CG	2.49	0.43
1:E:290:ILE:HG12	1:E:303:THR:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:PHE:CZ	1:F:47:ALA:HA	2.52	0.43
1:B:180:LEU:HD23	1:B:356:TYR:CZ	2.53	0.43
1:C:359:ALA:O	1:C:361:THR:N	2.51	0.43
1:E:90:PHE:O	1:E:92:ALA:N	2.51	0.43
1:D:122:GLN:HA	4:D:502:HOH:O	2.19	0.43
1:D:212:GLY:HA2	1:D:226:TRP:CH2	2.53	0.43
1:F:31:GLU:O	1:F:32:ILE:HD13	2.18	0.43
1:B:45:LYS:CG	1:B:49:GLU:OE2	2.66	0.43
1:E:106:THR:CG2	1:E:350:LYS:CD	2.96	0.43
1:F:135:VAL:HG22	1:F:278:ILE:HD13	2.00	0.43
1:B:128:GLN:NE2	3:B:401:NAD:H72N	2.12	0.43
1:B:358:SER:C	1:B:360:LYS:H	2.27	0.43
1:C:23:LEU:HD13	1:C:32:ILE:HD11	2.01	0.43
1:C:183:ILE:C	1:C:185:THR:N	2.74	0.43
1:E:82:HIS:CD2	1:E:98:CYS:SG	3.11	0.43
1:E:279:HIS:HB3	1:E:284:TYR:CE2	2.54	0.43
1:F:234:GLU:O	1:F:234:GLU:HG2	2.18	0.43
1:A:19:HIS:ND1	1:A:74:HIS:ND1	2.66	0.43
1:A:172:LYS:N	1:A:232:GLU:OE1	2.32	0.43
1:B:300:MET:HE3	1:F:304:LEU:HD23	2.01	0.43
1:F:99:GLU:O	1:F:125:ILE:HG23	2.19	0.43
1:A:14:ILE:HG21	1:A:99:GLU:CG	2.46	0.43
1:A:177:GLY:N	1:A:181:ILE:HD11	2.34	0.43
1:B:154:LYS:HE3	1:E:252:GLU:OE2	2.18	0.43
1:B:157:ALA:HA	1:B:264:GLU:HA	2.00	0.43
1:D:163:VAL:HG22	1:D:255:TRP:HB3	2.01	0.43
1:D:254:SER:OG	1:D:257:ILE:HB	2.19	0.43
1:E:87:ILE:HG23	1:E:88:ALA:N	2.33	0.43
1:F:303:THR:HG22	1:F:304:LEU:H	1.83	0.43
1:A:154:LYS:HE3	4:F:507:HOH:O	2.19	0.42
1:C:29:LEU:HD21	1:C:326:ARG:NH2	2.31	0.42
1:D:239:GLY:HA3	1:D:355:ILE:HD13	1.99	0.42
1:B:139:LYS:HE2	1:B:193:TRP:CE2	2.53	0.42
1:D:56:GLN:O	1:D:57:VAL:C	2.62	0.42
1:F:93:GLY:C	1:F:94:LYS:CG	2.92	0.42
1:F:160:ARG:HA	1:F:257:ILE:O	2.20	0.42
1:A:156:HIS:HB2	1:A:266:SER:HB2	2.01	0.42
1:A:261:ASP:OD2	1:A:263:ARG:NH2	2.52	0.42
1:D:14:ILE:HD12	1:D:14:ILE:HA	1.74	0.42
1:D:64:LEU:HD23	1:D:64:LEU:O	2.19	0.42
1:E:131:PHE:CD2	1:E:324:ASP:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:NZ	2:A:401:BGC:O4	2.52	0.42
1:B:14:ILE:HD12	1:B:14:ILE:HA	1.83	0.42
1:C:82:HIS:CD2	1:C:98:CYS:SG	3.12	0.42
1:D:242:LYS:NZ	4:D:505:HOH:O	2.47	0.42
1:D:319:GLU:OE2	1:D:319:GLU:HA	2.19	0.42
1:E:157:ALA:O	1:E:253:ALA:HA	2.19	0.42
1:F:15:ALA:HB1	1:F:20:PHE:CZ	2.54	0.42
1:F:139:LYS:HE2	1:F:193:TRP:CE2	2.54	0.42
1:A:14:ILE:HD12	1:A:14:ILE:HA	1.82	0.42
1:A:60:ASP:CG	1:A:63:GLU:N	2.70	0.42
1:A:128:GLN:C	1:A:130:ARG:H	2.28	0.42
1:D:179:PRO:HD2	1:D:234:GLU:CD	2.45	0.42
1:E:181:ILE:HG23	1:E:356:TYR:HE2	1.85	0.42
1:A:159:ARG:NH2	1:A:264:GLU:OE2	2.53	0.42
2:D:401:BGC:H3	3:D:402:NAD:C4N	2.49	0.42
1:E:4:LEU:HD11	1:E:332:ILE:HG22	2.00	0.42
1:B:9:ILE:HD12	1:B:73:VAL:CG1	2.45	0.42
1:B:90:PHE:O	1:B:92:ALA:N	2.52	0.42
1:C:106:THR:HG23	1:C:350:LYS:CG	2.50	0.42
1:D:32:ILE:CG2	1:D:35:PHE:CE1	3.03	0.42
1:E:83:SER:O	1:E:87:ILE:HB	2.19	0.42
1:F:35:PHE:CD2	1:F:47:ALA:CA	3.03	0.42
1:F:36:CYS:SG	1:F:37:ASP:N	2.92	0.42
1:F:79:ASN:HD22	1:F:82:HIS:CE1	2.38	0.42
1:F:130:ARG:HA	1:F:135:VAL:CG1	2.47	0.42
1:A:32:ILE:H	1:A:32:ILE:HG13	1.29	0.42
1:A:80:VAL:HG11	1:A:173:GLU:O	2.20	0.42
1:C:90:PHE:O	1:C:92:ALA:N	2.51	0.42
1:C:188:LEU:HD22	1:C:348:VAL:HG22	2.01	0.42
1:A:327:GLN:OE1	1:A:339:LEU:N	2.35	0.41
1:C:159:ARG:HH22	2:C:401:BGC:C5	2.32	0.41
1:E:175:GLN:O	1:E:181:ILE:HD11	2.20	0.41
1:F:86:THR:O	1:F:86:THR:HG22	2.20	0.41
1:A:332:ILE:O	1:A:333:GLN:C	2.63	0.41
1:B:36:CYS:HA	1:B:58:THR:O	2.20	0.41
1:B:180:LEU:HB3	1:B:356:TYR:OH	2.20	0.41
1:D:29:LEU:HD11	1:D:326:ARG:NH1	2.35	0.41
1:D:102:MET:HE3	1:D:125:ILE:HD11	2.02	0.41
1:E:124:THR:O	1:E:125:ILE:HD13	2.20	0.41
1:E:179:PRO:HA	1:E:182:ASP:HB3	2.02	0.41
1:A:222:LEU:HD23	1:A:223:PHE:CZ	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:HE2	1:C:193:TRP:NE1	2.36	0.41
1:C:304:LEU:HD21	1:E:298:GLN:OE1	2.20	0.41
1:D:157:ALA:HB1	1:D:183:ILE:HG13	2.02	0.41
1:F:134:GLU:HG2	1:F:135:VAL:N	2.35	0.41
1:B:282:MET:HA	1:B:282:MET:CE	2.35	0.41
1:D:8:ILE:HD12	1:D:74:HIS:HB2	2.02	0.41
1:D:101:PRO:O	1:D:102:MET:C	2.62	0.41
1:D:188:LEU:HD23	1:D:188:LEU:HA	1.82	0.41
1:E:80:VAL:HA	1:E:104:HIS:HE1	1.85	0.41
1:E:188:LEU:HD13	1:E:251:LEU:HD12	2.02	0.41
1:F:222:LEU:C	1:F:224:GLY:N	2.78	0.41
1:C:240:PHE:HB2	1:D:240:PHE:CD1	2.55	0.41
1:F:203:VAL:HG22	1:F:241:VAL:HG13	2.02	0.41
1:A:26:ASN:OD1	1:A:326:ARG:NE	2.54	0.41
1:A:100:LYS:HG3	1:A:186:HIS:CE1	2.56	0.41
1:A:327:GLN:HE21	1:A:327:GLN:HB3	1.66	0.41
1:C:130:ARG:HD3	1:C:193:TRP:CE3	2.55	0.41
1:D:29:LEU:CD1	1:D:326:ARG:HH12	2.33	0.41
1:E:100:LYS:O	1:E:102:MET:N	2.54	0.41
1:E:106:THR:CG2	1:E:350:LYS:CG	2.97	0.41
1:F:327:GLN:HE21	1:F:327:GLN:HB3	1.65	0.41
1:B:165:THR:HG22	1:B:226:TRP:HB3	2.03	0.41
1:D:36:CYS:SG	1:D:37:ASP:N	2.93	0.41
1:E:216:ASN:ND2	1:E:216:ASN:H	2.18	0.41
1:F:3:LYS:HB2	1:F:3:LYS:HZ3	1.86	0.41
1:A:128:GLN:C	1:A:130:ARG:N	2.78	0.41
1:A:179:PRO:HB3	1:A:255:TRP:CD1	2.56	0.41
1:D:248:THR:C	1:D:249:ILE:HD12	2.45	0.41
1:A:160:ARG:HD3	1:F:299:LEU:HD13	2.02	0.41
1:C:130:ARG:HD3	1:C:193:TRP:CD2	2.55	0.41
1:D:28:ASP:CG	1:D:29:LEU:HD12	2.46	0.41
1:D:44:GLU:O	1:D:45:LYS:C	2.64	0.41
1:D:91:GLU:C	1:D:93:GLY:H	2.29	0.41
1:D:134:GLU:HG2	1:D:135:VAL:N	2.35	0.41
1:D:179:PRO:HB3	1:D:255:TRP:CD1	2.56	0.41
1:D:195:MET:CE	1:D:249:ILE:HD11	2.50	0.41
1:F:154:LYS:HB2	1:F:268:THR:HB	2.03	0.41
1:F:178:GLY:HA3	1:F:179:PRO:HD2	1.75	0.41
1:C:22:ALA:HA	1:C:322:THR:HG22	2.03	0.41
1:C:100:LYS:HZ1	1:C:101:PRO:HG3	1.83	0.41
1:C:252:GLU:OE1	1:D:154:LYS:HE3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:ALA:O	1:F:253:ALA:HA	2.20	0.41
1:D:365:LYS:HD3	1:D:366:PHE:N	2.37	0.40
1:E:124:THR:HG22	1:E:328:TRP:CZ3	2.56	0.40
1:F:125:ILE:HG13	1:F:345:ALA:CB	2.51	0.40
1:A:159:ARG:HE	1:A:282:MET:HE2	1.86	0.40
1:C:37:ASP:C	1:C:39:GLN:N	2.79	0.40
1:C:95:HIS:ND1	1:C:122:GLN:HB2	2.37	0.40
1:E:139:LYS:HE2	1:E:193:TRP:CE2	2.55	0.40
1:F:24:LYS:O	1:F:25:ASN:C	2.64	0.40
1:F:100:LYS:HD2	1:F:185:THR:HG21	2.03	0.40
1:A:116:TRP:CD1	1:A:123:PHE:HB2	2.57	0.40
1:A:130:ARG:O	1:A:136:MET:HE2	2.21	0.40
1:A:141:SER:OG	1:D:296:ASN:ND2	2.53	0.40
1:A:171:ASP:CG	1:A:174:ALA:H	2.28	0.40
1:A:251:LEU:HD23	1:A:251:LEU:C	2.47	0.40
1:A:268:THR:HG23	1:A:277:GLU:HB3	2.04	0.40
1:A:325:ASN:ND2	1:A:325:ASN:C	2.78	0.40
1:A:341:LYS:HA	1:A:342:PRO:HD3	1.95	0.40
1:C:25:ASN:ND2	1:C:322:THR:HG21	2.35	0.40
1:D:3:LYS:NZ	1:D:28:ASP:HA	2.36	0.40
1:D:43:ALA:O	1:D:47:ALA:N	2.40	0.40
1:F:183:ILE:HD11	1:F:254:SER:O	2.22	0.40
1:F:336:THR:OG1	1:F:337:GLU:N	2.54	0.40
1:C:106:THR:HG21	1:C:350:LYS:HG2	2.04	0.40
1:E:216:ASN:O	1:E:219:GLU:HB2	2.20	0.40
1:F:93:GLY:HA3	1:F:94:LYS:NZ	2.36	0.40
1:A:218:PRO:HA	1:A:226:TRP:CZ3	2.55	0.40
1:C:31:GLU:HB2	1:C:52:ALA:HB2	2.04	0.40
1:C:124:THR:C	1:C:125:ILE:HD13	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/367 (92%)	296 (88%)	28 (8%)	12 (4%)	2	2
1	B	350/367 (95%)	332 (95%)	16 (5%)	2 (1%)	21	30
1	C	342/367 (93%)	321 (94%)	18 (5%)	3 (1%)	14	20
1	D	342/367 (93%)	314 (92%)	22 (6%)	6 (2%)	6	8
1	E	347/367 (95%)	326 (94%)	16 (5%)	5 (1%)	9	12
1	F	344/367 (94%)	312 (91%)	29 (8%)	3 (1%)	14	20
All	All	2061/2202 (94%)	1901 (92%)	129 (6%)	31 (2%)	8	11

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ALA
1	A	28	ASP
1	A	58	THR
1	D	51	GLY
1	D	100	LYS
1	E	88	ALA
1	E	90	PHE
1	E	100	LYS
1	A	360	LYS
1	C	360	LYS
1	D	45	LYS
1	D	53	GLU
1	F	52	ALA
1	F	118	LYS
1	A	50	PHE
1	B	358	SER
1	E	89	ALA
1	F	102	MET
1	A	64	LEU
1	A	68	PRO
1	A	87	ILE
1	E	358	SER
1	C	91	GLU
1	C	100	LYS
1	D	358	SER
1	B	89	ALA
1	D	57	VAL
1	A	78	PRO
1	A	120	GLY
1	A	12	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	93	GLY

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	259/294 (88%)	240 (93%)	19 (7%)	13	21
1	B	275/294 (94%)	274 (100%)	1 (0%)	84	92
1	C	276/294 (94%)	271 (98%)	5 (2%)	51	71
1	D	267/294 (91%)	257 (96%)	10 (4%)	30	49
1	E	275/294 (94%)	268 (98%)	7 (2%)	42	62
1	F	265/294 (90%)	246 (93%)	19 (7%)	13	21
All	All	1617/1764 (92%)	1556 (96%)	61 (4%)	29	47

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	9	ILE
1	A	14	ILE
1	A	17	GLN
1	A	23	LEU
1	A	24	LYS
1	A	28	ASP
1	A	30	ASN
1	A	32	ILE
1	A	33	VAL
1	A	49	GLU
1	A	60	ASP
1	A	61	TYR
1	A	63	GLU
1	A	81	SER
1	A	113	VAL
1	A	114	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	116	TRP
1	A	161	ARG
1	B	100	LYS
1	C	91	GLU
1	C	94	LYS
1	C	99	GLU
1	C	111	LYS
1	C	303	THR
1	D	3	LYS
1	D	38	ILE
1	D	40	ILE
1	D	100	LYS
1	D	102	MET
1	D	106	THR
1	D	118	LYS
1	D	172	LYS
1	D	348	VAL
1	D	362	ASN
1	E	14	ILE
1	E	38	ILE
1	E	53	GLU
1	E	87	ILE
1	E	91	GLU
1	E	94	LYS
1	E	362	ASN
1	F	60	ASP
1	F	86	THR
1	F	91	GLU
1	F	94	LYS
1	F	99	GLU
1	F	100	LYS
1	F	116	TRP
1	F	150	ILE
1	F	158	VAL
1	F	159	ARG
1	F	173	GLU
1	F	196	ASN
1	F	202	SER
1	F	214	LYS
1	F	226	TRP
1	F	235	ASP
1	F	259	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	332	ILE
1	F	361	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	67	ASN
1	A	79	ASN
1	A	122	GLN
1	A	128	GLN
1	A	325	ASN
1	B	128	GLN
1	C	16	ASN
1	C	25	ASN
1	C	39	GLN
1	C	82	HIS
1	C	128	GLN
1	D	39	GLN
1	D	79	ASN
1	D	196	ASN
1	E	79	ASN
1	E	104	HIS
1	E	196	ASN
1	E	216	ASN
1	E	296	ASN
1	E	362	ASN
1	F	30	ASN
1	F	79	ASN
1	F	128	GLN
1	F	129	ASN
1	F	196	ASN
1	F	197	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	NAD	D	402	-	46,48,48	0.59	1 (2%)	64,73,73	0.56	0
2	BGC	C	401	-	12,12,12	1.43	2 (16%)	17,17,17	1.43	3 (17%)
2	BGC	D	401	-	12,12,12	1.31	1 (8%)	17,17,17	1.04	2 (11%)
3	NAD	E	402	-	46,48,48	4.27	25 (54%)	64,73,73	2.38	25 (39%)
3	NAD	F	402	-	46,48,48	4.06	21 (45%)	64,73,73	2.20	14 (21%)
2	BGC	A	401	-	12,12,12	0.78	0	17,17,17	1.19	2 (11%)
3	NAD	C	402	-	46,48,48	4.14	22 (47%)	64,73,73	2.24	20 (31%)
2	BGC	F	401	-	12,12,12	1.32	1 (8%)	17,17,17	0.81	0
2	BGC	E	401	-	12,12,12	1.28	1 (8%)	17,17,17	0.79	0
3	NAD	A	402	-	46,48,48	2.20	15 (32%)	64,73,73	1.55	8 (12%)
3	NAD	B	401	-	46,48,48	3.93	20 (43%)	64,73,73	2.18	15 (23%)

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	NAD	D	402	-	-	4/30/62/62	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	401	-	-	2/2/22/22	0/1/1/1
2	BGC	D	401	-	-	2/2/22/22	0/1/1/1
3	NAD	E	402	-	-	7/30/62/62	0/5/5/5
3	NAD	F	402	-	-	11/30/62/62	0/5/5/5
2	BGC	A	401	-	-	2/2/22/22	0/1/1/1
3	NAD	C	402	-	-	10/30/62/62	0/5/5/5
2	BGC	F	401	-	-	2/2/22/22	0/1/1/1
2	BGC	E	401	-	-	2/2/22/22	0/1/1/1
3	NAD	A	402	-	-	8/30/62/62	0/5/5/5
3	NAD	B	401	-	-	13/30/62/62	0/5/5/5

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	NAD	O4D-C1D	-10.39	1.27	1.40
3	E	402	NAD	O4D-C1D	-10.37	1.27	1.40
3	F	402	NAD	O4D-C1D	-10.33	1.27	1.40
3	B	401	NAD	O4D-C1D	-10.21	1.27	1.40
3	E	402	NAD	PN-O3	9.96	1.70	1.59
3	C	402	NAD	PN-O3	9.91	1.70	1.59
3	F	402	NAD	PN-O3	9.82	1.70	1.59
3	B	401	NAD	C3B-C4B	-9.26	1.29	1.53
3	E	402	NAD	C3B-C4B	-9.20	1.29	1.53
3	F	402	NAD	C3B-C4B	-8.95	1.30	1.53
3	C	402	NAD	C3B-C4B	-8.93	1.30	1.53
3	F	402	NAD	C7N-N7N	8.81	1.49	1.33
3	E	402	NAD	C7N-N7N	8.75	1.49	1.33
3	B	401	NAD	C7N-N7N	8.65	1.48	1.33
3	C	402	NAD	C7N-N7N	8.53	1.48	1.33
3	B	401	NAD	PN-O3	8.43	1.68	1.59
3	F	402	NAD	C3D-C4D	-8.35	1.31	1.53
3	B	401	NAD	C3D-C4D	-8.31	1.31	1.53
3	E	402	NAD	O4B-C4B	8.08	1.63	1.45
3	F	402	NAD	O4D-C4D	7.96	1.62	1.45
3	C	402	NAD	O4B-C4B	7.86	1.62	1.45
3	E	402	NAD	C3D-C4D	-7.84	1.33	1.53
3	C	402	NAD	O4D-C4D	7.73	1.62	1.45
3	E	402	NAD	O4D-C4D	7.50	1.61	1.45
3	B	401	NAD	O4D-C4D	7.39	1.61	1.45
3	F	402	NAD	O4B-C4B	7.37	1.61	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAD	O4B-C4B	7.36	1.61	1.45
3	C	402	NAD	C3D-C4D	-7.32	1.34	1.53
3	C	402	NAD	O3D-C3D	7.31	1.61	1.43
3	E	402	NAD	O3D-C3D	6.74	1.59	1.43
3	A	402	NAD	O4D-C1D	-6.58	1.32	1.40
3	E	402	NAD	C6A-N6A	6.20	1.50	1.34
3	C	402	NAD	C6A-N6A	6.10	1.49	1.34
3	B	401	NAD	C6A-N6A	5.91	1.49	1.34
3	F	402	NAD	C6A-N6A	5.70	1.48	1.34
3	E	402	NAD	C4N-C3N	-5.58	1.31	1.39
3	A	402	NAD	C4N-C3N	-5.45	1.31	1.39
3	C	402	NAD	PA-O3	5.21	1.65	1.59
3	C	402	NAD	C3N-C7N	5.15	1.58	1.50
3	E	402	NAD	C3N-C7N	5.15	1.58	1.50
3	F	402	NAD	C3N-C7N	5.07	1.58	1.50
3	B	401	NAD	C3N-C7N	4.99	1.58	1.50
3	F	402	NAD	PA-O3	4.82	1.64	1.59
3	E	402	NAD	PA-O3	4.78	1.64	1.59
3	F	402	NAD	O3D-C3D	4.42	1.53	1.43
3	F	402	NAD	O4B-C1B	-4.28	1.32	1.42
3	B	401	NAD	O3D-C3D	4.26	1.53	1.43
3	B	401	NAD	O4B-C1B	-4.16	1.32	1.42
3	E	402	NAD	C5N-C4N	4.15	1.46	1.38
3	A	402	NAD	C6N-N1N	-4.15	1.25	1.35
3	C	402	NAD	O4B-C1B	-4.09	1.32	1.42
3	E	402	NAD	O4B-C1B	-3.92	1.32	1.42
3	A	402	NAD	C5N-C4N	-3.66	1.32	1.38
3	B	401	NAD	PA-O3	3.66	1.63	1.59
3	A	402	NAD	PN-O3	-3.64	1.55	1.59
2	C	401	BGC	O5-C1	3.60	1.51	1.42
2	F	401	BGC	O5-C1	3.54	1.51	1.42
2	D	401	BGC	O5-C1	3.39	1.51	1.42
3	A	402	NAD	PA-O3	-3.38	1.55	1.59
3	F	402	NAD	C2N-N1N	3.36	1.38	1.35
2	E	401	BGC	O5-C1	3.30	1.50	1.42
3	F	402	NAD	O3B-C3B	3.24	1.51	1.43
3	C	402	NAD	C2N-N1N	3.16	1.38	1.35
3	C	402	NAD	O3B-C3B	3.13	1.50	1.43
3	E	402	NAD	O3B-C3B	3.00	1.50	1.43
3	C	402	NAD	C2A-N1A	2.98	1.39	1.33
3	A	402	NAD	PA-O2A	-2.97	1.41	1.55
3	B	401	NAD	C2N-N1N	2.95	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAD	O3B-C3B	2.93	1.50	1.43
3	A	402	NAD	O7N-C7N	-2.90	1.18	1.24
3	E	402	NAD	C2N-N1N	2.89	1.38	1.35
3	B	401	NAD	C8A-N9A	-2.86	1.32	1.37
3	E	402	NAD	PA-O5B	2.85	1.70	1.59
3	B	401	NAD	C5A-C4A	-2.85	1.34	1.39
3	E	402	NAD	C2A-N1A	2.84	1.39	1.33
3	A	402	NAD	C2N-N1N	-2.76	1.31	1.35
3	E	402	NAD	O2B-C2B	-2.76	1.36	1.43
3	F	402	NAD	C5A-C4A	-2.76	1.34	1.39
3	F	402	NAD	C2A-N1A	2.74	1.38	1.33
3	B	401	NAD	C2A-N1A	2.71	1.38	1.33
3	C	402	NAD	C8A-N9A	-2.63	1.33	1.37
3	D	402	NAD	C2N-N1N	2.63	1.37	1.35
3	E	402	NAD	C8A-N9A	-2.59	1.33	1.37
3	A	402	NAD	PN-O2N	-2.58	1.43	1.55
3	F	402	NAD	C8A-N9A	-2.58	1.33	1.37
3	F	402	NAD	O2B-C2B	-2.54	1.36	1.43
3	A	402	NAD	C2N-C3N	-2.53	1.35	1.39
3	C	402	NAD	PA-O5B	2.51	1.69	1.59
3	C	402	NAD	O2B-C2B	-2.49	1.36	1.43
3	B	401	NAD	O7N-C7N	-2.47	1.19	1.24
3	A	402	NAD	PA-O1A	-2.45	1.42	1.50
3	B	401	NAD	O2B-C2B	-2.44	1.36	1.43
3	E	402	NAD	C5B-C4B	2.43	1.58	1.51
3	E	402	NAD	O7N-C7N	-2.38	1.19	1.24
3	A	402	NAD	PN-O5D	-2.35	1.50	1.59
3	C	402	NAD	O7N-C7N	-2.34	1.19	1.24
3	F	402	NAD	O7N-C7N	-2.34	1.19	1.24
3	E	402	NAD	C8A-N7A	2.26	1.36	1.31
3	B	401	NAD	C8A-N7A	2.25	1.36	1.31
3	E	402	NAD	C5A-C4A	-2.24	1.35	1.39
3	C	402	NAD	C5A-N7A	-2.20	1.35	1.39
3	C	402	NAD	C5A-C4A	-2.19	1.35	1.39
3	C	402	NAD	C5B-C4B	2.18	1.58	1.51
3	F	402	NAD	C8A-N7A	2.14	1.35	1.31
3	A	402	NAD	C5A-C4A	-2.12	1.35	1.39
2	C	401	BGC	O5-C5	2.09	1.49	1.44
3	E	402	NAD	C5A-N7A	-2.08	1.35	1.39
3	A	402	NAD	C8A-N9A	-2.06	1.34	1.37
3	F	402	NAD	PA-O5B	2.04	1.67	1.59

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAD	C4A-N9A-C1B	-7.08	110.08	126.63
3	F	402	NAD	C4A-N9A-C1B	-7.01	110.24	126.63
3	A	402	NAD	O2B-C2B-C1B	-6.48	87.80	110.10
3	B	401	NAD	N3A-C2A-N1A	-5.70	119.96	128.58
3	F	402	NAD	N3A-C2A-N1A	-5.58	120.14	128.58
3	E	402	NAD	C5A-C4A-N3A	-5.57	119.05	126.72
3	B	401	NAD	N9A-C8A-N7A	-5.49	106.15	113.94
3	F	402	NAD	N9A-C8A-N7A	-5.46	106.19	113.94
3	B	401	NAD	C1B-N9A-C8A	5.46	139.21	127.09
3	F	402	NAD	C1B-N9A-C8A	5.40	139.08	127.09
3	C	402	NAD	C4A-N9A-C1B	-5.30	114.23	126.63
3	C	402	NAD	N3A-C2A-N1A	-5.24	120.66	128.58
3	A	402	NAD	O2N-PN-O3	-5.18	93.27	107.27
3	E	402	NAD	C4A-N9A-C1B	-5.05	114.81	126.63
3	E	402	NAD	N3A-C2A-N1A	-5.02	120.98	128.58
3	E	402	NAD	N9A-C8A-N7A	-4.86	107.04	113.94
3	C	402	NAD	C5A-C4A-N3A	-4.82	120.08	126.72
3	F	402	NAD	N6A-C6A-N1A	-4.81	107.67	118.38
3	B	401	NAD	C4A-N9A-C8A	4.71	110.68	105.74
3	F	402	NAD	C4A-N9A-C8A	4.70	110.67	105.74
3	E	402	NAD	N6A-C6A-N1A	-4.67	107.98	118.38
3	B	401	NAD	N6A-C6A-N1A	-4.62	108.08	118.38
3	C	402	NAD	N9A-C8A-N7A	-4.59	107.43	113.94
3	E	402	NAD	C4D-O4D-C1D	-4.54	105.77	109.92
3	C	402	NAD	N6A-C6A-N1A	-4.41	108.55	118.38
3	B	401	NAD	C5A-C4A-N3A	-4.38	120.68	126.72
3	F	402	NAD	C5A-C4A-N3A	-4.30	120.79	126.72
3	C	402	NAD	C1B-N9A-C8A	4.08	136.16	127.09
3	E	402	NAD	C1B-N9A-C8A	4.02	136.02	127.09
3	E	402	NAD	N3A-C4A-N9A	4.01	133.99	127.17
2	C	401	BGC	O5-C5-C4	3.96	116.83	109.70
3	C	402	NAD	N3A-C4A-N9A	3.90	133.81	127.17
3	A	402	NAD	O3B-C3B-C4B	-3.85	100.01	111.08
3	E	402	NAD	C5A-C6A-N6A	3.83	132.76	123.29
3	C	402	NAD	C4A-N9A-C8A	3.69	109.61	105.74
3	E	402	NAD	C5A-N7A-C8A	3.62	109.14	103.45
3	C	402	NAD	C5A-C6A-N6A	3.58	132.16	123.29
3	E	402	NAD	C2N-C3N-C4N	3.56	122.39	118.26
3	B	401	NAD	C5A-C6A-N6A	3.55	132.07	123.29
3	F	402	NAD	C5A-C6A-N6A	3.55	132.06	123.29
3	C	402	NAD	C2D-C3D-C4D	-3.50	95.84	102.61
3	C	402	NAD	C4D-O4D-C1D	-3.50	106.72	109.92
3	F	402	NAD	N3A-C4A-N9A	3.49	133.10	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAD	N3A-C4A-N9A	3.45	133.03	127.17
3	E	402	NAD	C6N-N1N-C2N	-3.36	119.02	121.88
3	E	402	NAD	C2D-C3D-C4D	-3.33	96.18	102.61
3	C	402	NAD	C6N-N1N-C2N	-3.28	119.09	121.88
3	E	402	NAD	C4A-N9A-C8A	3.27	109.17	105.74
3	C	402	NAD	O3D-C3D-C2D	3.24	122.20	111.82
3	B	401	NAD	C5A-N7A-C8A	3.23	108.53	103.45
3	F	402	NAD	C5A-N7A-C8A	3.20	108.48	103.45
3	E	402	NAD	C2A-N3A-C4A	3.19	119.63	111.83
3	F	402	NAD	C4D-O4D-C1D	-3.15	107.04	109.92
3	F	402	NAD	C2A-N3A-C4A	3.13	119.48	111.83
3	B	401	NAD	C2A-N3A-C4A	3.12	119.46	111.83
3	A	402	NAD	O4B-C4B-C3B	-3.07	99.05	105.15
3	E	402	NAD	C6A-C5A-C4A	3.04	121.33	117.18
3	A	402	NAD	O2N-PN-O1N	3.04	126.60	112.44
3	C	402	NAD	C5A-N7A-C8A	3.03	108.22	103.45
3	C	402	NAD	C2A-N3A-C4A	2.94	119.02	111.83
3	E	402	NAD	C5N-C4N-C3N	-2.87	117.55	120.36
3	E	402	NAD	O3D-C3D-C2D	2.87	121.01	111.82
3	A	402	NAD	C1B-N9A-C8A	-2.77	120.94	127.09
3	B	401	NAD	C3N-C7N-N7N	2.60	120.95	117.74
3	C	402	NAD	C3B-C2B-C1B	2.59	106.36	101.46
3	C	402	NAD	C6A-C5A-C4A	2.58	120.70	117.18
3	E	402	NAD	C3B-C2B-C1B	2.57	106.33	101.46
3	E	402	NAD	C2B-C3B-C4B	2.54	107.53	102.61
3	E	402	NAD	C4A-C5A-N7A	-2.53	107.69	110.58
3	C	402	NAD	C2B-C1B-N9A	-2.51	107.06	113.30
3	F	402	NAD	C6N-N1N-C2N	-2.50	119.75	121.88
2	D	401	BGC	C6-C5-C4	-2.47	106.94	113.02
3	E	402	NAD	O4D-C4D-C3D	2.39	109.89	105.15
2	A	401	BGC	C4-C3-C2	2.32	114.91	110.83
3	C	402	NAD	C2B-C3B-C4B	2.31	107.07	102.61
3	C	402	NAD	O7N-C7N-N7N	-2.28	119.32	122.62
3	A	402	NAD	C4A-N9A-C1B	2.28	131.96	126.63
2	C	401	BGC	C1-O5-C5	2.26	118.02	113.65
3	A	402	NAD	C2B-C1B-N9A	-2.20	107.84	113.30
3	B	401	NAD	C6N-N1N-C2N	-2.19	120.02	121.88
3	B	401	NAD	C2B-C3B-C4B	2.18	106.82	102.61
2	C	401	BGC	C3-C4-C5	2.18	114.18	110.23
3	B	401	NAD	O7N-C7N-N7N	-2.14	119.53	122.62
2	A	401	BGC	O1-C1-O5	-2.12	104.13	110.41
2	D	401	BGC	O5-C5-C4	2.11	113.51	109.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	NAD	O4B-C1B-C2B	-2.11	102.11	106.62
3	F	402	NAD	O4B-C4B-C3B	2.08	109.27	105.15
3	E	402	NAD	O4B-C1B-N9A	2.02	111.97	108.09
3	E	402	NAD	C3N-C7N-N7N	2.01	120.22	117.74

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAD	O4D-C1D-N1N-C6N
3	A	402	NAD	C2D-C1D-N1N-C2N
3	A	402	NAD	C2D-C1D-N1N-C6N
3	B	401	NAD	C5B-O5B-PA-O2A
3	B	401	NAD	C5B-O5B-PA-O3
3	B	401	NAD	O4D-C1D-N1N-C2N
3	B	401	NAD	O4D-C1D-N1N-C6N
3	B	401	NAD	C2D-C1D-N1N-C2N
3	B	401	NAD	C2D-C1D-N1N-C6N
3	C	402	NAD	C5D-O5D-PN-O2N
3	C	402	NAD	O4D-C4D-C5D-O5D
3	C	402	NAD	O4D-C1D-N1N-C2N
3	C	402	NAD	O4D-C1D-N1N-C6N
3	C	402	NAD	C2D-C1D-N1N-C2N
3	D	402	NAD	O4D-C1D-N1N-C2N
3	D	402	NAD	O4D-C1D-N1N-C6N
3	D	402	NAD	C2D-C1D-N1N-C2N
3	D	402	NAD	C2D-C1D-N1N-C6N
3	E	402	NAD	O4D-C1D-N1N-C6N
3	F	402	NAD	C5B-O5B-PA-O2A
3	F	402	NAD	C5B-O5B-PA-O3
3	F	402	NAD	O4D-C1D-N1N-C6N
2	F	401	BGC	C4-C5-C6-O6
2	E	401	BGC	C4-C5-C6-O6
2	A	401	BGC	O5-C5-C6-O6
2	F	401	BGC	O5-C5-C6-O6
2	A	401	BGC	C4-C5-C6-O6
2	D	401	BGC	C4-C5-C6-O6
3	C	402	NAD	C3D-C4D-C5D-O5D
3	F	402	NAD	O4D-C4D-C5D-O5D
3	F	402	NAD	C3D-C4D-C5D-O5D
2	E	401	BGC	O5-C5-C6-O6
2	D	401	BGC	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	401	BGC	O5-C5-C6-O6
3	A	402	NAD	C3B-C4B-C5B-O5B
3	A	402	NAD	O4B-C4B-C5B-O5B
3	F	402	NAD	O4B-C4B-C5B-O5B
3	F	402	NAD	C3B-C4B-C5B-O5B
3	B	401	NAD	O4B-C4B-C5B-O5B
2	C	401	BGC	C4-C5-C6-O6
3	B	401	NAD	C3B-C4B-C5B-O5B
3	E	402	NAD	C3D-C4D-C5D-O5D
3	E	402	NAD	O4D-C4D-C5D-O5D
3	B	401	NAD	PN-O3-PA-O5B
3	F	402	NAD	PN-O3-PA-O5B
3	B	401	NAD	C2B-C1B-N9A-C8A
3	F	402	NAD	C2B-C1B-N9A-C8A
3	A	402	NAD	C2B-C1B-N9A-C8A
3	B	401	NAD	C5B-O5B-PA-O1A
3	C	402	NAD	C5D-O5D-PN-O3
3	C	402	NAD	C5D-O5D-PN-O1N
3	E	402	NAD	C5D-O5D-PN-O1N
3	F	402	NAD	C5B-O5B-PA-O1A
3	B	401	NAD	PA-O3-PN-O2N
3	E	402	NAD	PA-O3-PN-O2N
3	C	402	NAD	C2D-C1D-N1N-C6N
3	A	402	NAD	O4D-C1D-N1N-C2N
3	E	402	NAD	O4D-C1D-N1N-C2N
3	F	402	NAD	O4D-C1D-N1N-C2N
3	C	402	NAD	C2B-C1B-N9A-C8A
3	B	401	NAD	PA-O3-PN-O1N
3	E	402	NAD	PA-O3-PN-O1N
3	A	402	NAD	O4B-C1B-N9A-C8A

There are no ring outliers.

10 monomers are involved in 51 short contacts:

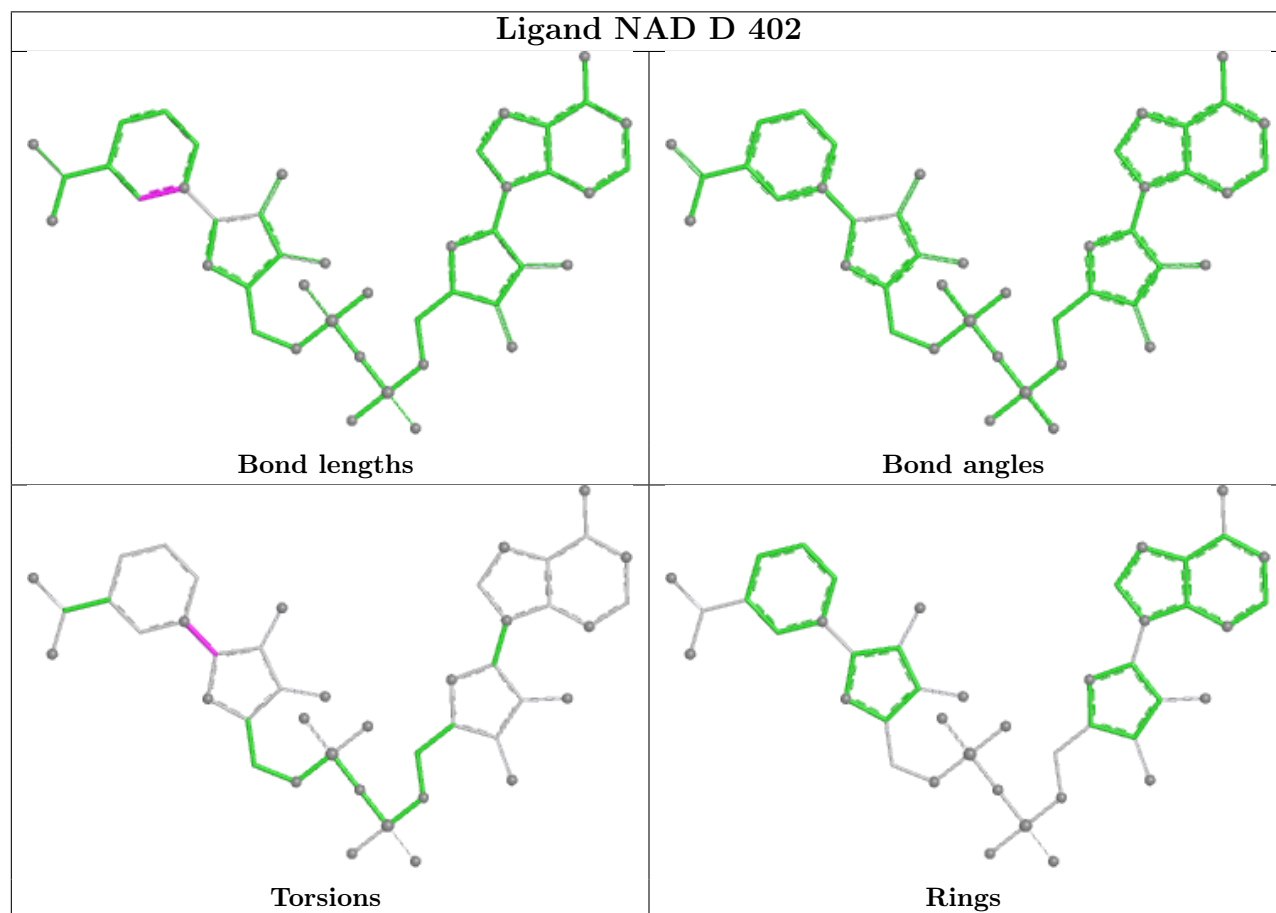
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	NAD	6	0
2	C	401	BGC	1	0
2	D	401	BGC	5	0
3	E	402	NAD	6	0
3	F	402	NAD	10	0
2	A	401	BGC	5	0
3	C	402	NAD	7	0

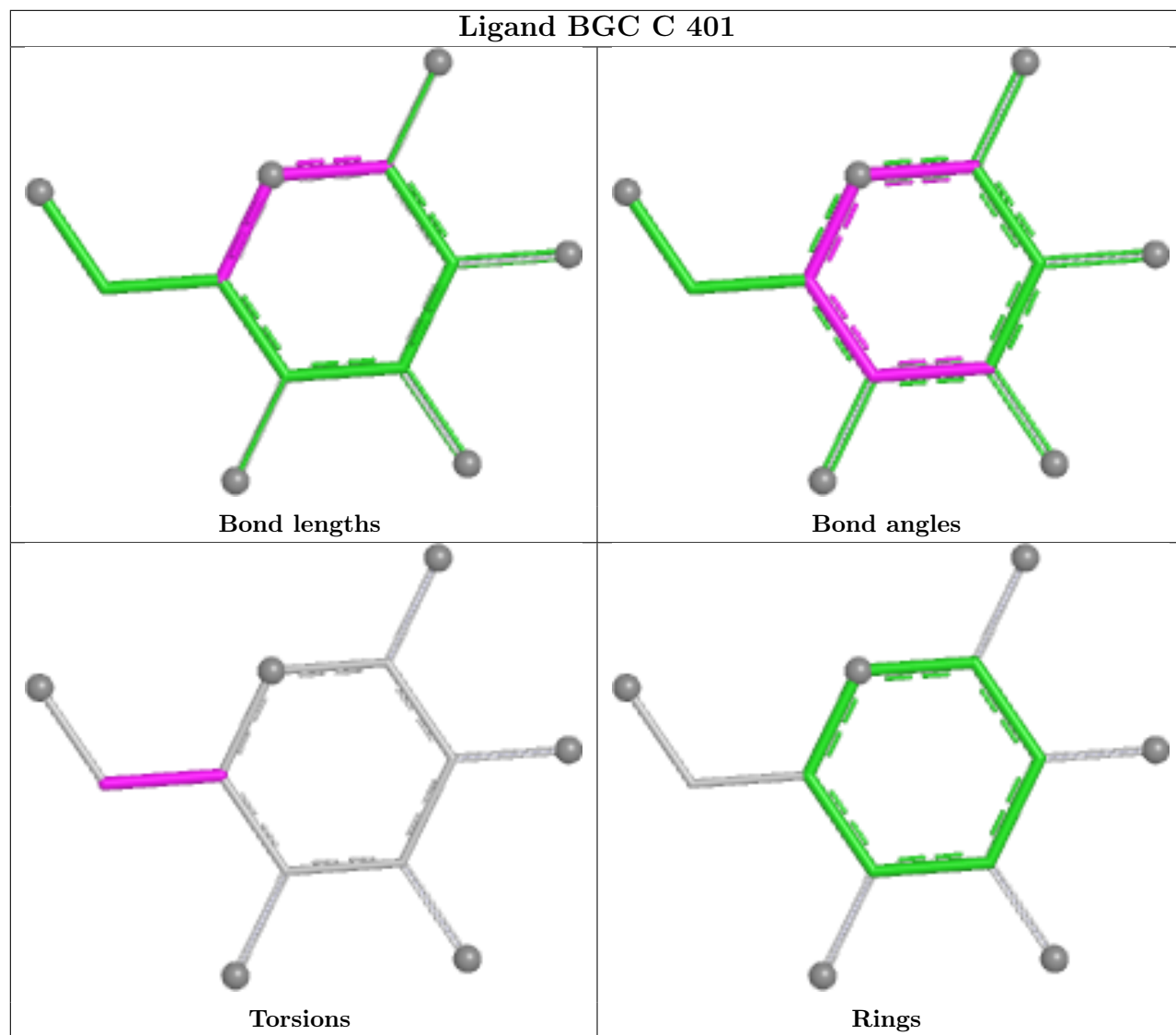
Continued on next page...

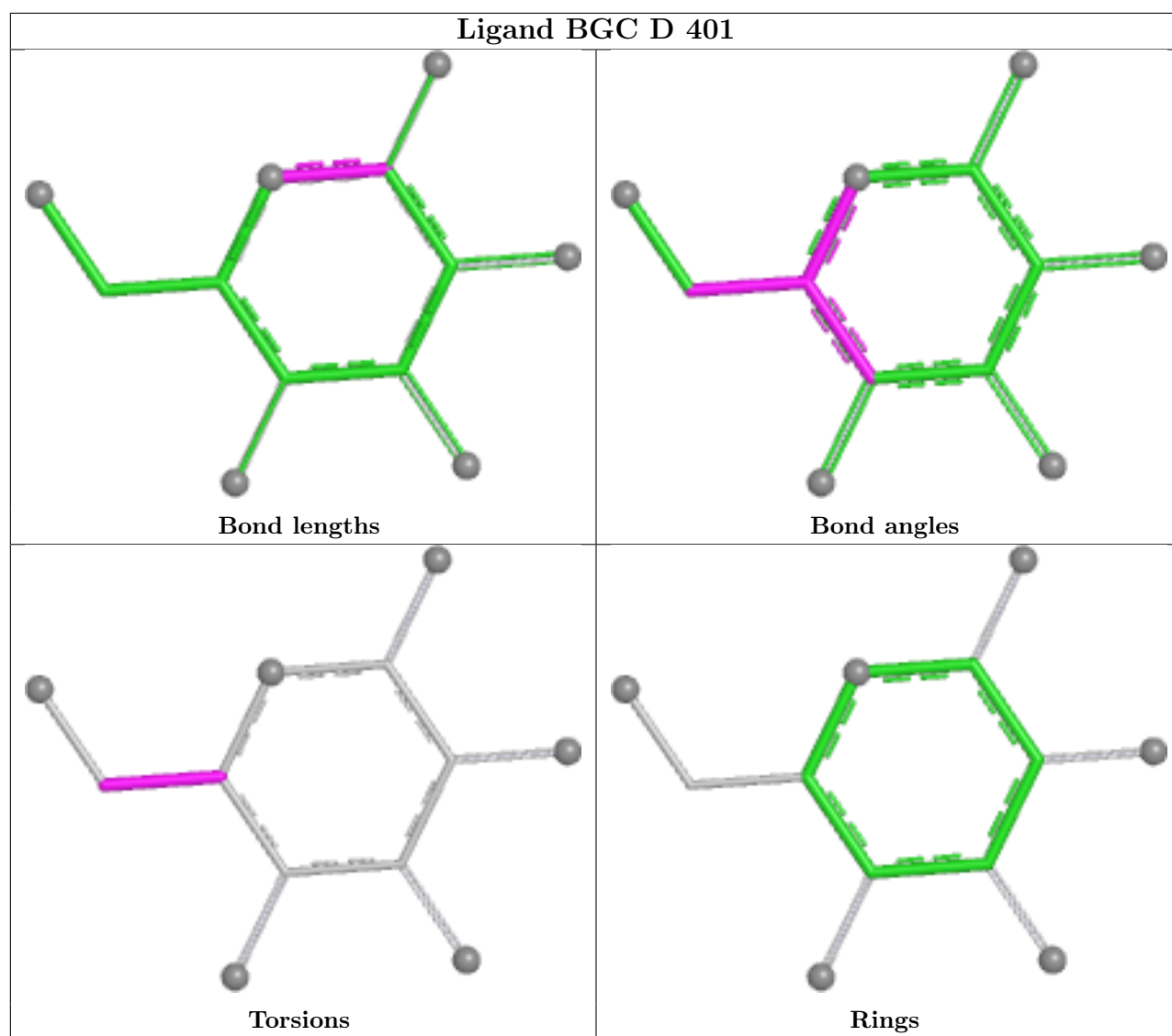
Continued from previous page...

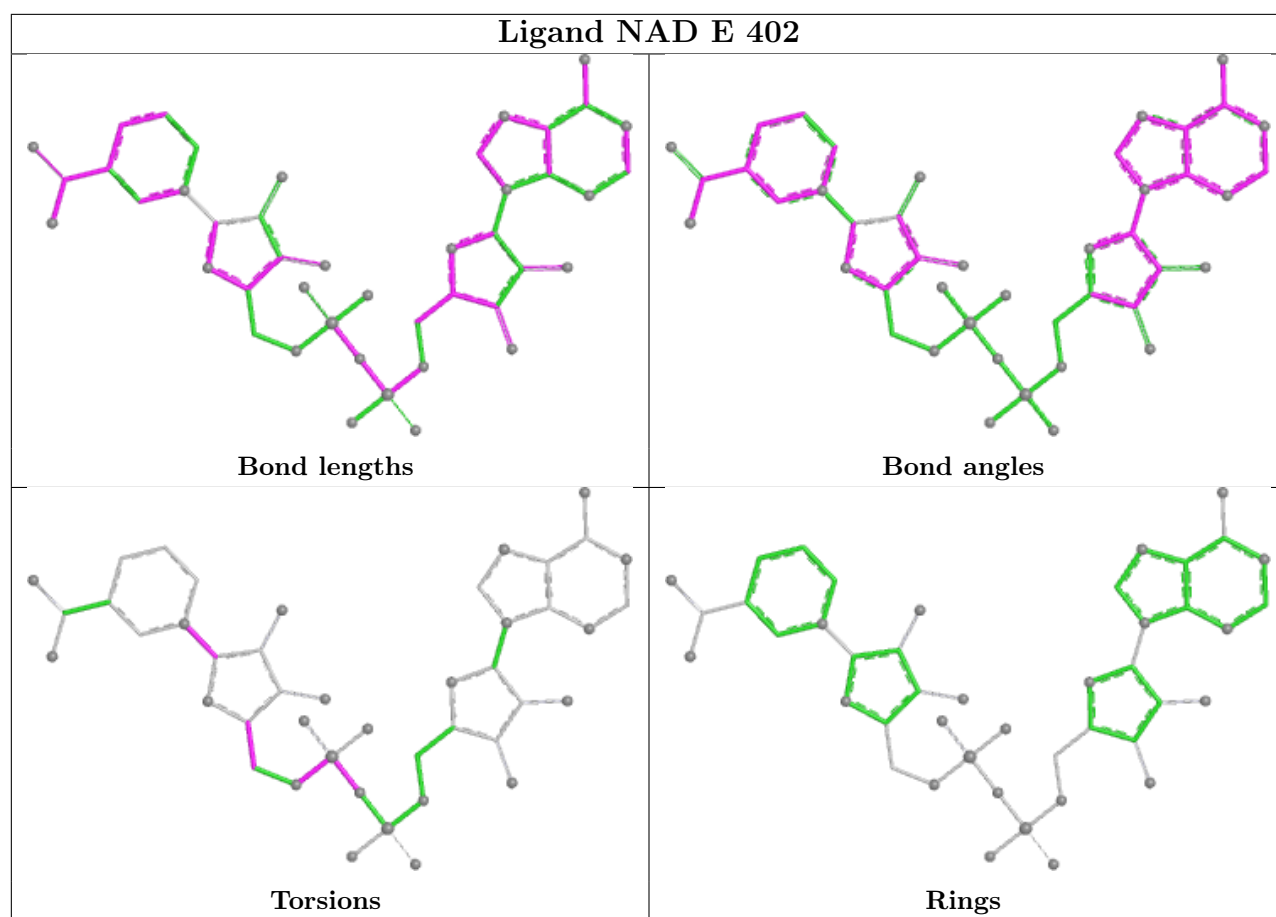
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	BGC	1	0
3	A	402	NAD	7	0
3	B	401	NAD	6	0

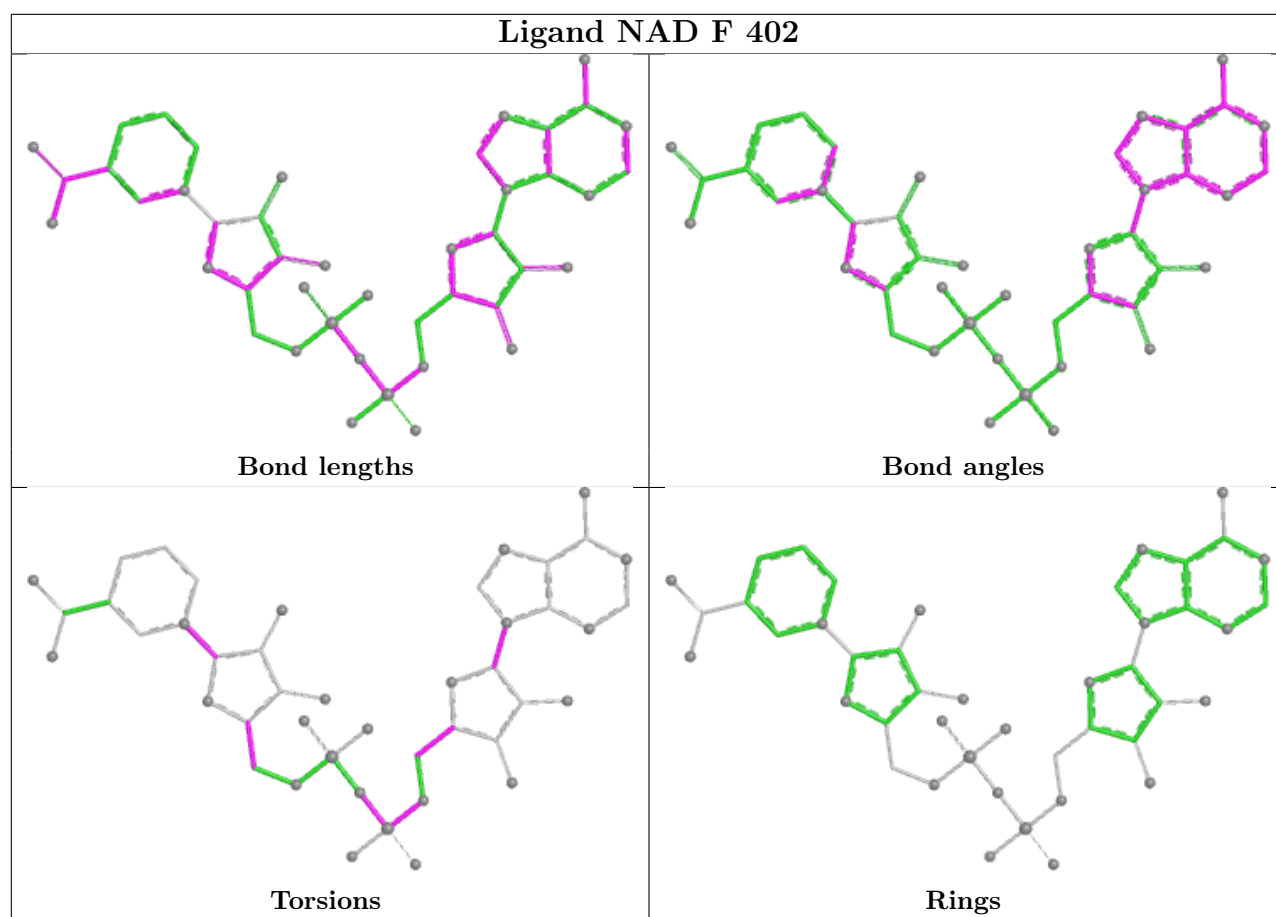
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

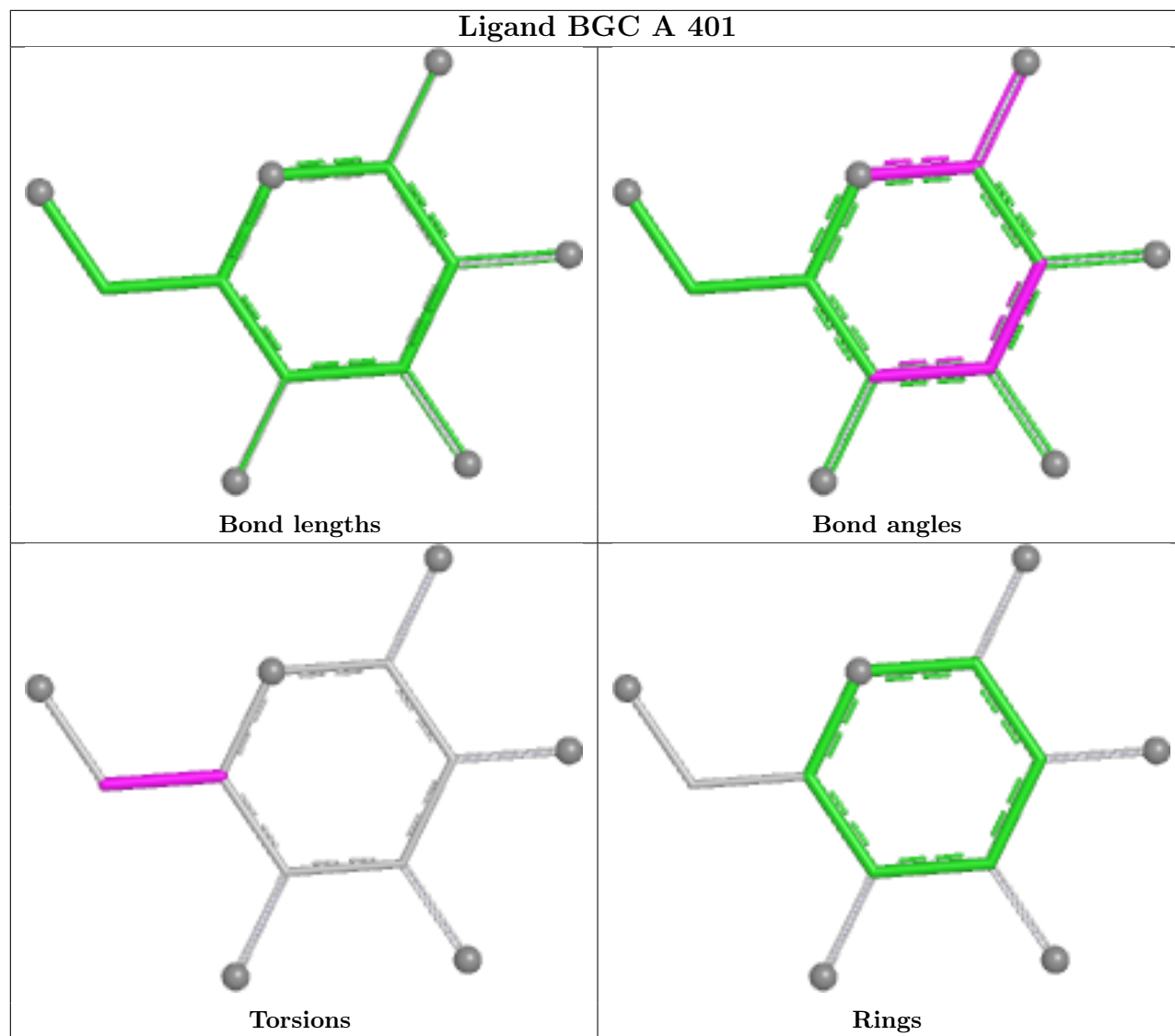


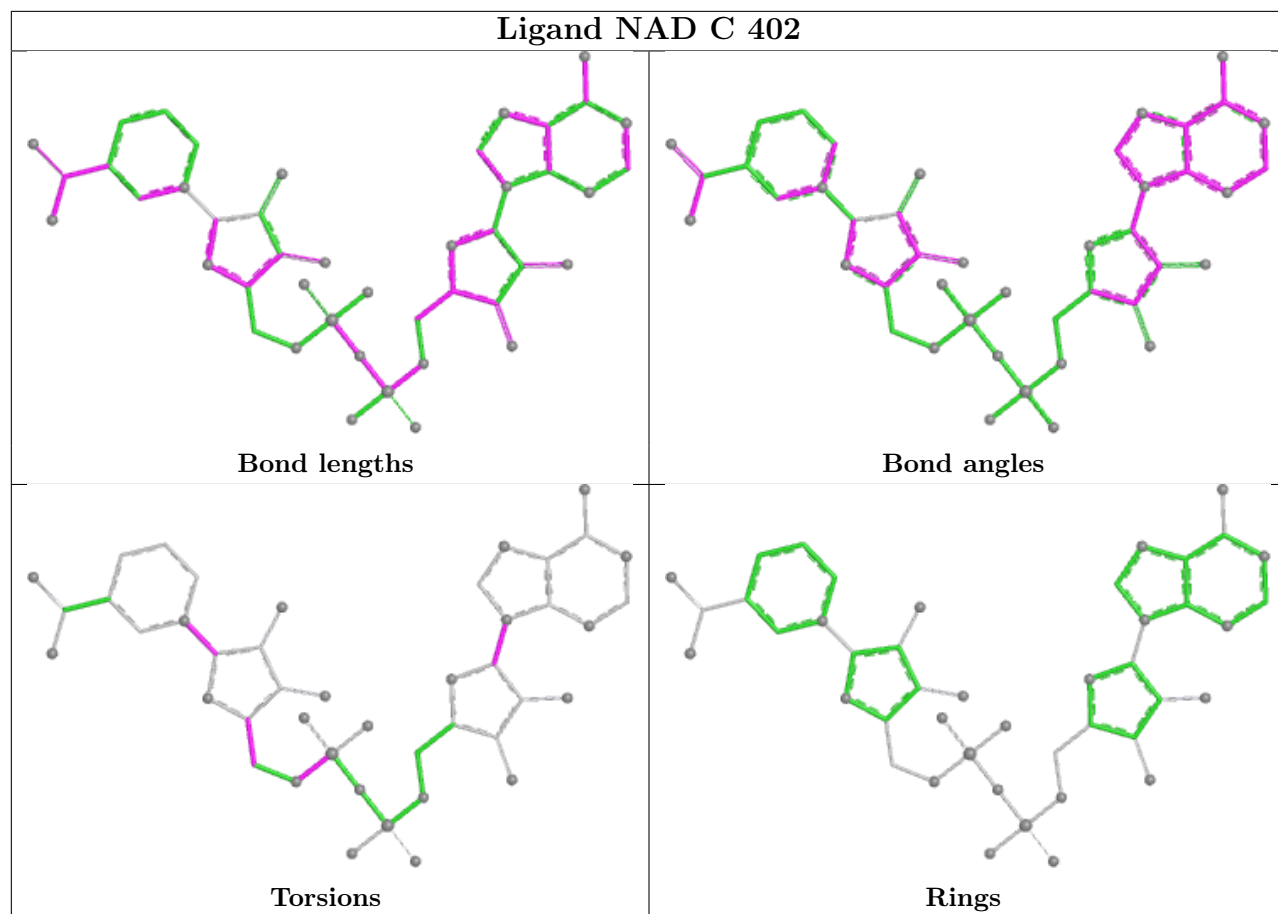


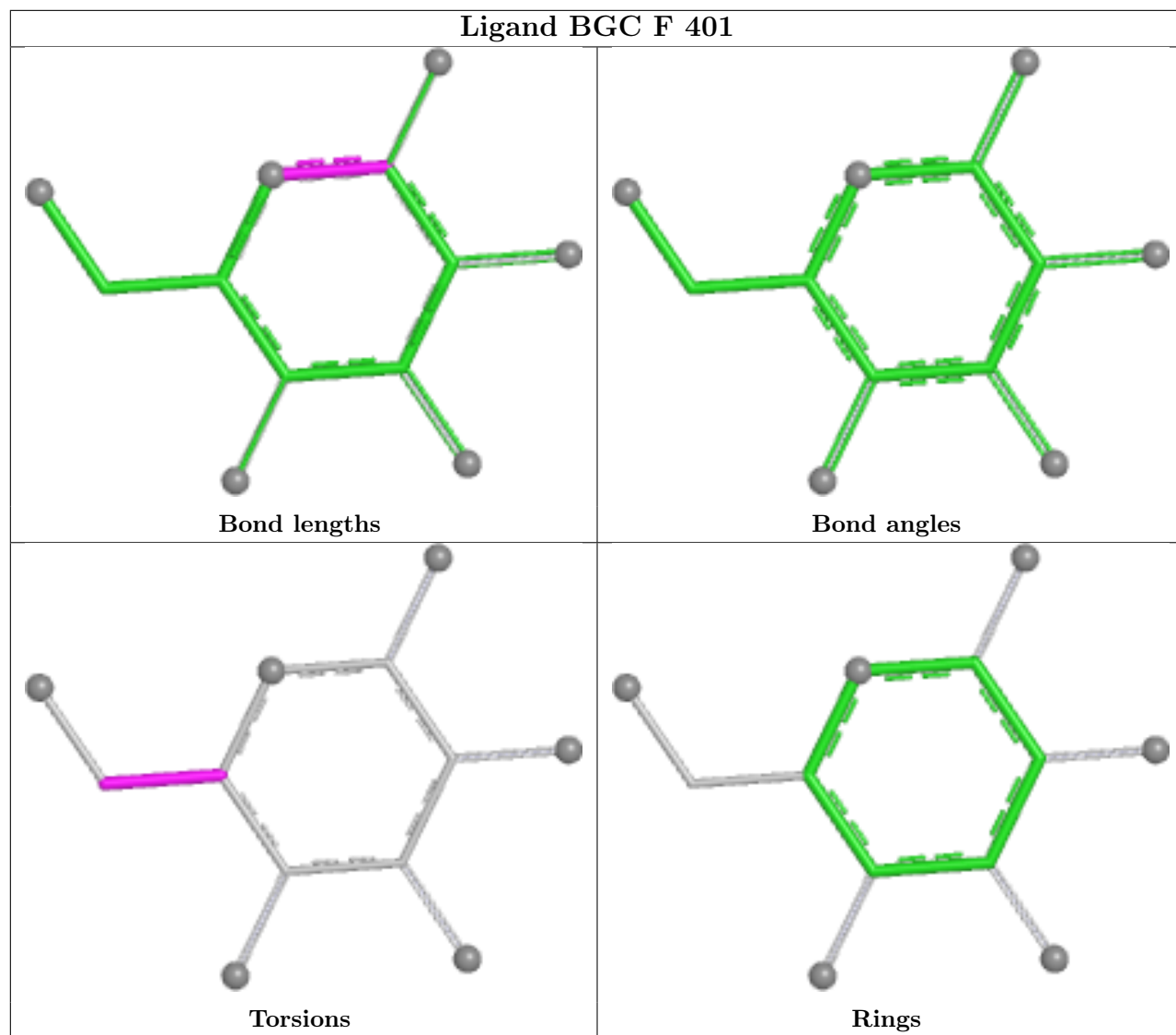


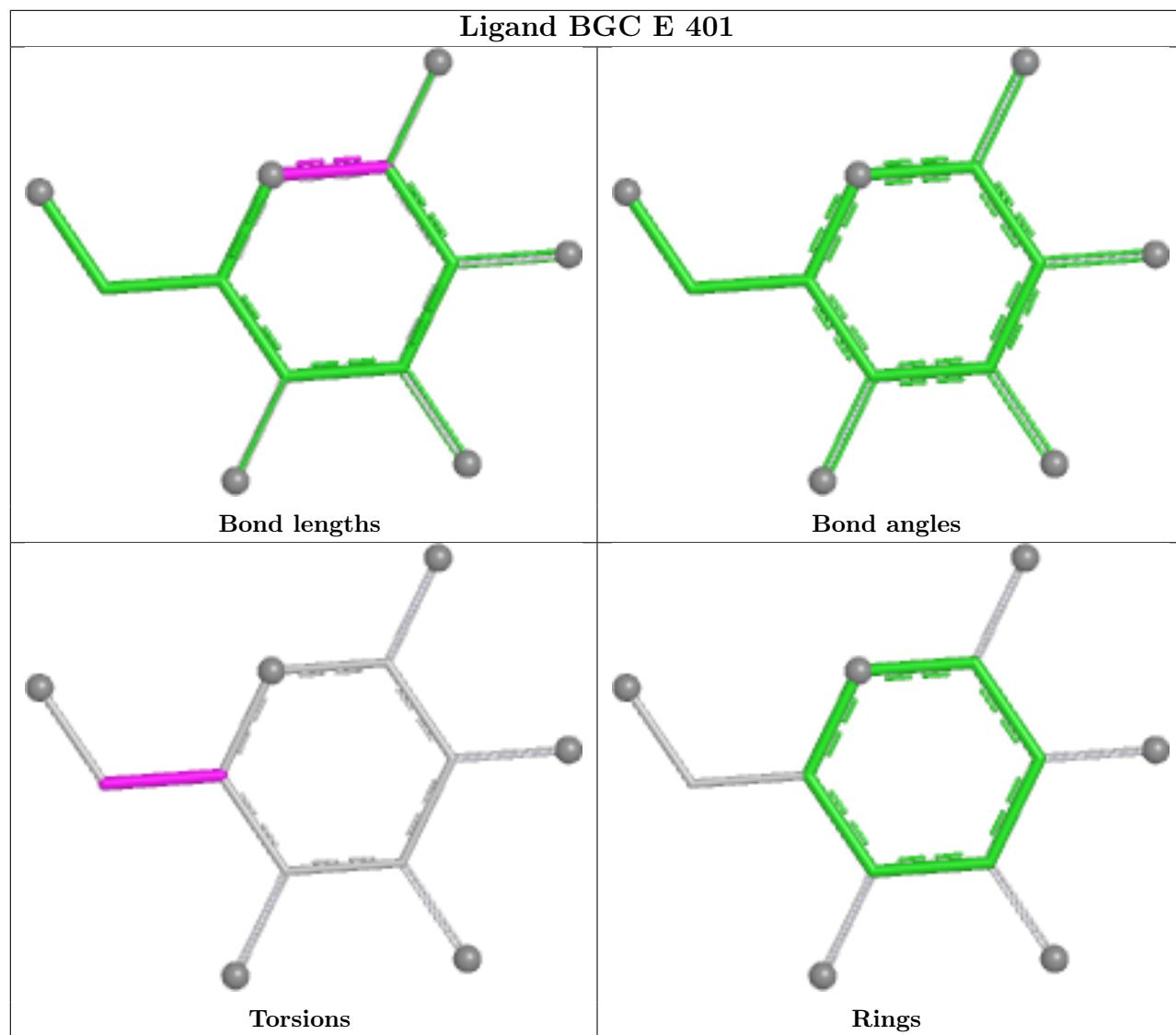


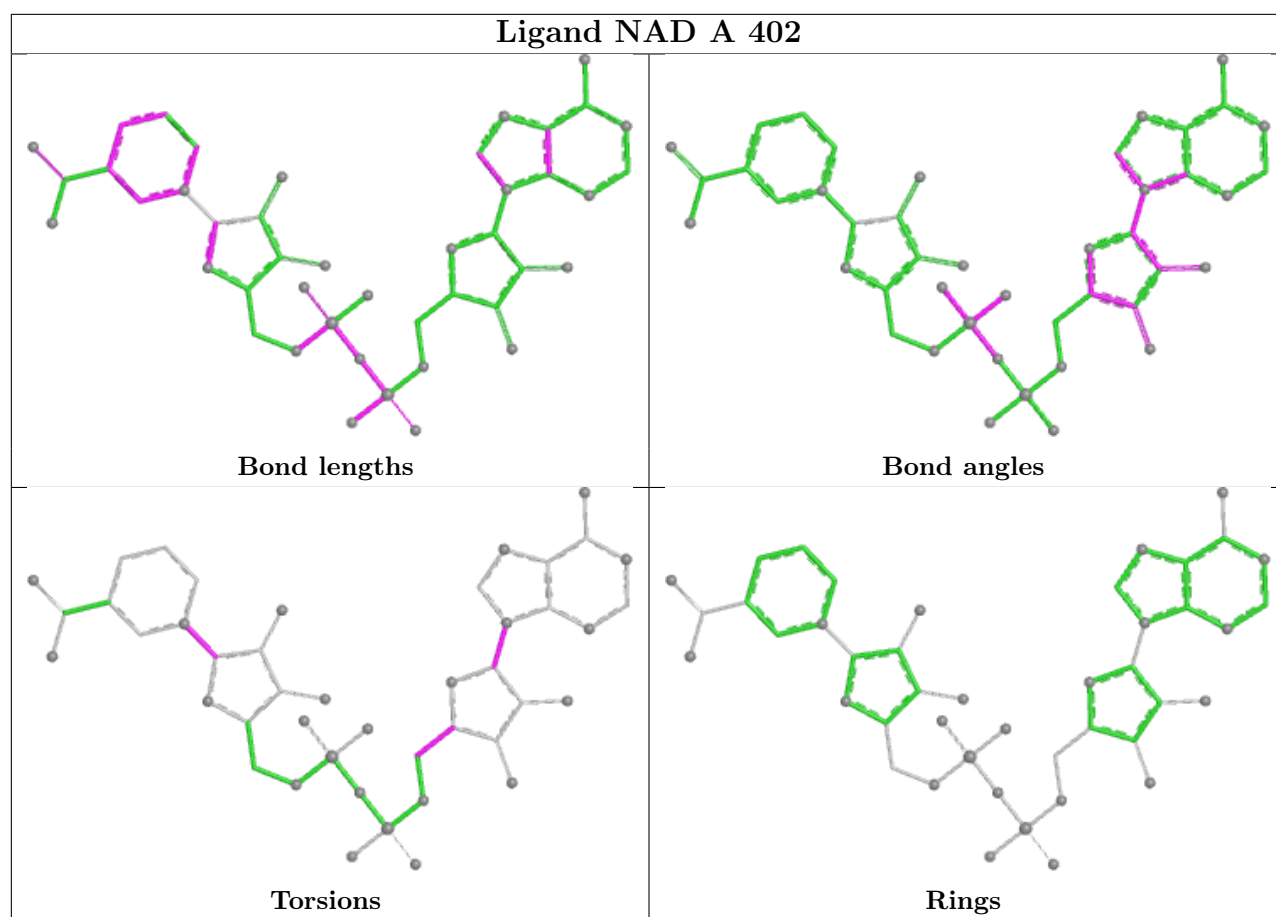


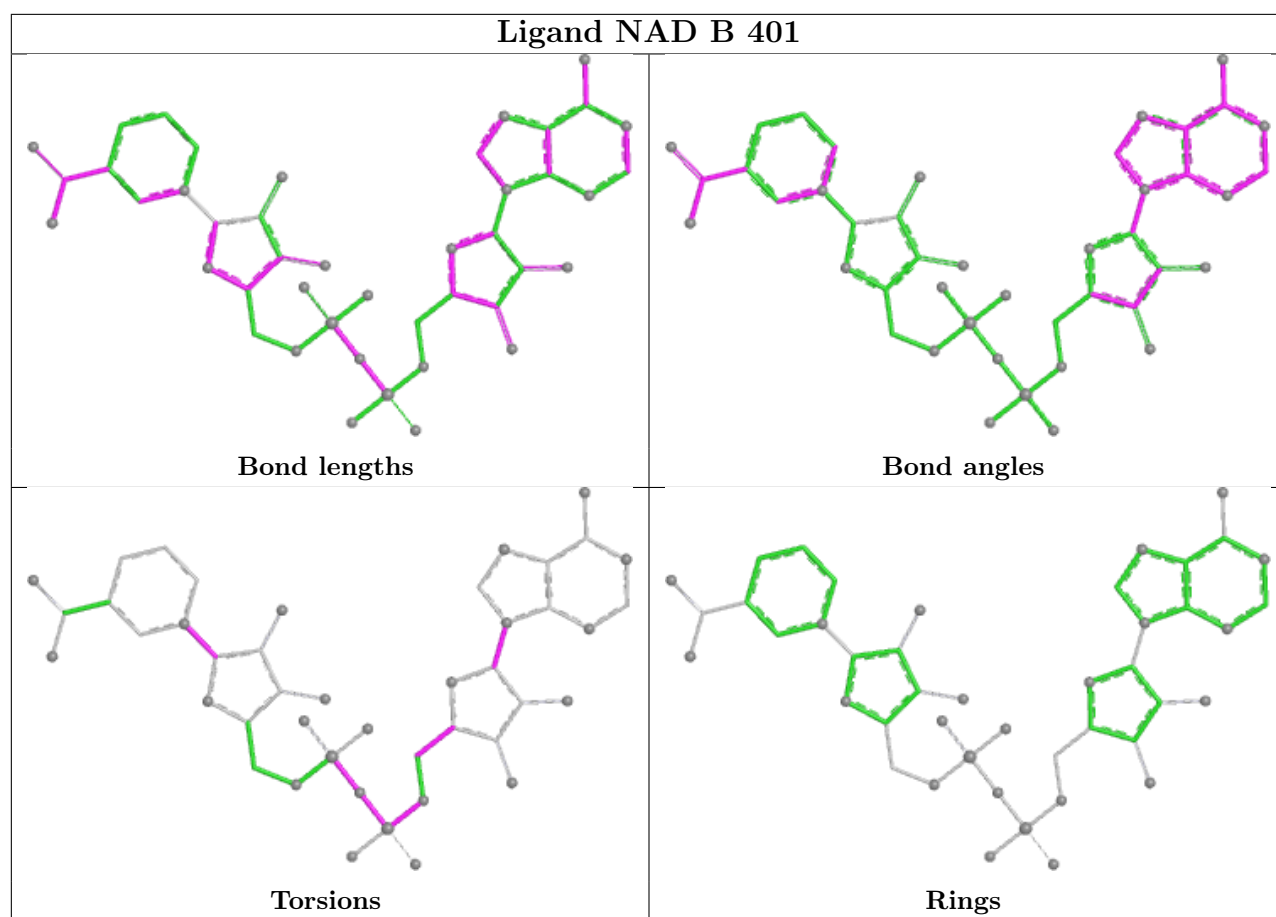












5.7 Other polymers [i](#)

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	344/367 (93%)	0.90	61 (17%) 4 3	30, 55, 110, 120	0
1	B	354/367 (96%)	0.19	11 (3%) 51 48	30, 46, 67, 94	0
1	C	350/367 (95%)	0.42	21 (6%) 27 24	30, 52, 75, 108	0
1	D	350/367 (95%)	0.66	39 (11%) 10 8	30, 54, 95, 126	0
1	E	353/367 (96%)	0.23	13 (3%) 45 41	30, 49, 69, 105	0
1	F	350/367 (95%)	0.80	38 (10%) 10 8	30, 56, 95, 109	0
All	All	2101/2202 (95%)	0.53	183 (8%) 16 13	30, 51, 93, 126	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	89	ALA	12.5
1	D	88	ALA	7.6
1	E	88	ALA	6.7
1	F	52	ALA	6.7
1	D	52	ALA	6.5
1	F	86	THR	6.0
1	F	91	GLU	5.7
1	C	359	ALA	5.3
1	A	359	ALA	5.3
1	C	52	ALA	5.3
1	B	90	PHE	5.1
1	F	100	LYS	5.1
1	F	33	VAL	5.1
1	A	59	ALA	4.9
1	A	55	ALA	4.9
1	C	100	LYS	4.9
1	F	88	ALA	4.8
1	F	93	GLY	4.6
1	F	89	ALA	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	90	PHE	4.5
1	F	92	ALA	4.4
1	A	43	ALA	4.4
1	A	66	ALA	4.4
1	F	85	ILE	4.2
1	F	101	PRO	4.1
1	D	33	VAL	4.1
1	A	9	ILE	4.1
1	A	64	LEU	4.0
1	D	35	PHE	4.0
1	A	33	VAL	3.9
1	F	99	GLU	3.9
1	F	57	VAL	3.8
1	A	57	VAL	3.8
1	C	92	ALA	3.8
1	F	226	TRP	3.8
1	A	61	TYR	3.7
1	A	88	ALA	3.7
1	C	78	PRO	3.7
1	D	92	ALA	3.7
1	E	92	ALA	3.7
1	A	85	ILE	3.6
1	B	100	LYS	3.6
1	A	68	PRO	3.6
1	F	130	ARG	3.6
1	E	89	ALA	3.6
1	A	100	LYS	3.6
1	F	90	PHE	3.6
1	A	168	VAL	3.5
1	B	359	ALA	3.5
1	C	0	GLY	3.4
1	A	65	LEU	3.4
1	B	92	ALA	3.4
1	D	47	ALA	3.4
1	D	59	ALA	3.4
1	A	76	CYS	3.4
1	A	56	GLN	3.4
1	A	96	VAL	3.4
1	D	55	ALA	3.4
1	D	358	SER	3.4
1	A	8	ILE	3.3
1	A	32	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	87	ILE	3.3
1	D	51	GLY	3.3
1	E	359	ALA	3.3
1	F	87	ILE	3.3
1	D	38	ILE	3.2
1	F	94	LYS	3.2
1	A	92	ALA	3.2
1	E	101	PRO	3.2
1	C	226	TRP	3.1
1	D	40	ILE	3.1
1	A	4	LEU	3.1
1	D	57	VAL	3.1
1	F	71	GLU	3.1
1	A	1	MET	3.1
1	E	366	PHE	3.1
1	F	131	PHE	3.0
1	C	358	SER	3.0
1	D	226	TRP	3.0
1	D	359	ALA	3.0
1	C	77	THR	2.9
1	F	361	THR	2.9
1	C	33	VAL	2.9
1	A	60	ASP	2.9
1	A	94	LYS	2.9
1	B	87	ILE	2.9
1	A	20	PHE	2.8
1	D	2	SER	2.8
1	A	84	GLU	2.8
1	A	75	VAL	2.8
1	A	90	PHE	2.8
1	A	15	ALA	2.8
1	D	43	ALA	2.8
1	A	87	ILE	2.7
1	F	358	SER	2.7
1	D	282	MET	2.7
1	A	358	SER	2.7
1	F	3	LYS	2.7
1	D	89	ALA	2.7
1	A	14	ILE	2.7
1	F	129	ASN	2.7
1	C	366	PHE	2.6
1	A	149	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	86	THR	2.6
1	A	10	GLY	2.6
1	E	93	GLY	2.6
1	D	101	PRO	2.6
1	A	31	GLU	2.6
1	B	101	PRO	2.6
1	A	167	GLY	2.5
1	D	32	ILE	2.5
1	F	62	LYS	2.5
1	C	102	MET	2.5
1	B	358	SER	2.5
1	D	69	GLU	2.5
1	F	32	ILE	2.5
1	A	19	HIS	2.5
1	A	70	VAL	2.4
1	D	46	ALA	2.4
1	A	83	SER	2.4
1	A	91	GLU	2.4
1	A	11	CYS	2.4
1	F	64	LEU	2.4
1	F	50	PHE	2.4
1	A	44	GLU	2.4
1	A	361	THR	2.4
1	F	65	LEU	2.4
1	F	169	PHE	2.4
1	F	96	VAL	2.3
1	A	30	ASN	2.3
1	A	47	ALA	2.3
1	A	71	GLU	2.3
1	A	89	ALA	2.3
1	C	55	ALA	2.3
1	F	53	GLU	2.3
1	C	86	THR	2.3
1	C	31	GLU	2.3
1	A	58	THR	2.3
1	F	166	TRP	2.3
1	D	53	GLU	2.3
1	D	91	GLU	2.3
1	F	59	ALA	2.3
1	D	11	CYS	2.3
1	F	68	PRO	2.3
1	E	358	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	91	GLU	2.2
1	C	101	PRO	2.2
1	A	77	THR	2.2
1	E	0	GLY	2.2
1	F	222	LEU	2.2
1	C	53	GLU	2.2
1	D	44	GLU	2.2
1	A	62	LYS	2.2
1	F	8	ILE	2.2
1	E	226	TRP	2.2
1	C	54	GLY	2.2
1	D	10	GLY	2.2
1	D	85	ILE	2.2
1	A	159	ARG	2.2
1	D	50	PHE	2.2
1	E	360	LYS	2.2
1	C	76	CYS	2.1
1	D	36	CYS	2.1
1	C	360	LYS	2.1
1	A	116	TRP	2.1
1	A	336	THR	2.1
1	A	6	ILE	2.1
1	D	8	ILE	2.1
1	A	169	PHE	2.1
1	D	90	PHE	2.1
1	D	22	ALA	2.1
1	E	83	SER	2.1
1	D	20	PHE	2.1
1	D	39	GLN	2.1
1	A	48	ALA	2.1
1	A	13	GLY	2.1
1	D	7	GLY	2.1
1	F	31	GLU	2.1
1	B	194	CYS	2.1
1	D	80	VAL	2.0
1	A	29	LEU	2.0
1	D	21	PRO	2.0
1	B	85	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

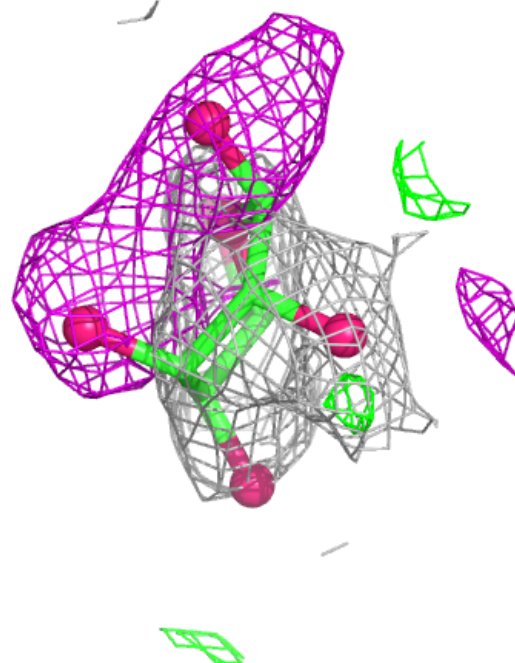
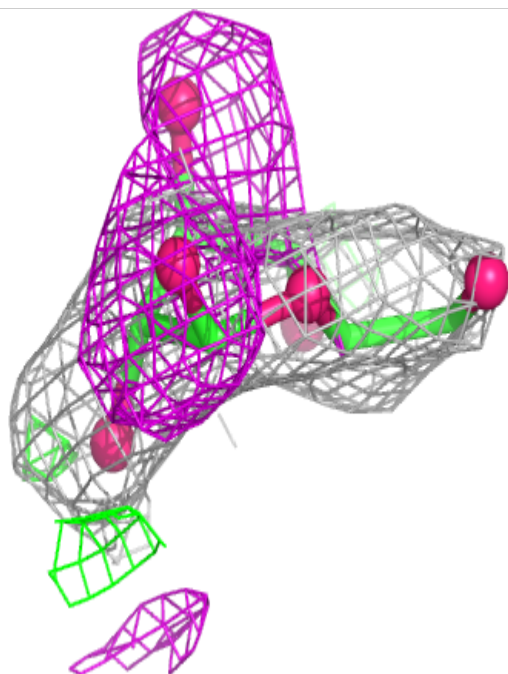
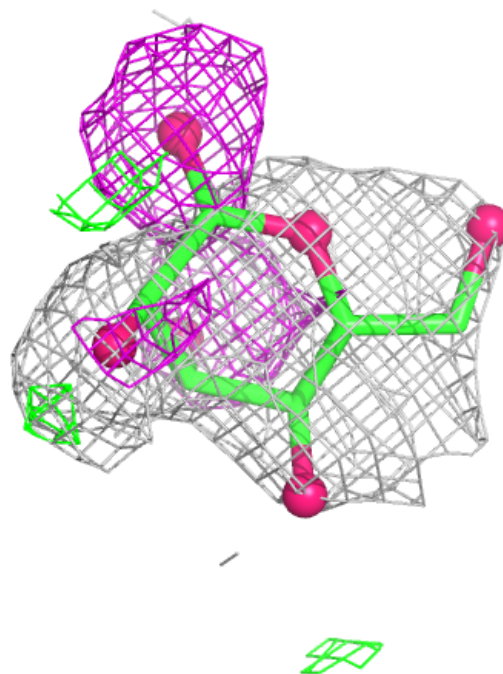
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	A	401	12/12	0.59	0.19	64,71,74,75	0
2	BGC	F	401	12/12	0.71	0.20	99,101,101,101	0
2	BGC	C	401	12/12	0.76	0.18	75,77,84,87	0
3	NAD	A	402	44/44	0.79	0.14	57,80,104,106	0
2	BGC	E	401	12/12	0.81	0.14	56,63,66,68	0
2	BGC	D	401	12/12	0.82	0.14	78,82,83,84	0
3	NAD	D	402	44/44	0.86	0.14	49,70,79,86	0
3	NAD	F	402	44/44	0.89	0.11	56,65,75,76	0
3	NAD	E	402	44/44	0.92	0.12	44,50,64,70	0
3	NAD	C	402	44/44	0.92	0.10	44,56,63,65	0
3	NAD	B	401	44/44	0.95	0.09	44,46,49,53	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.

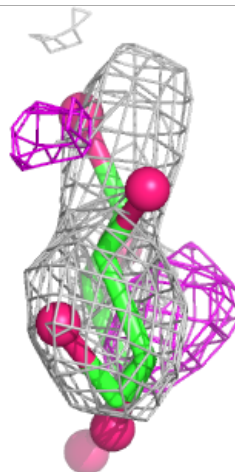
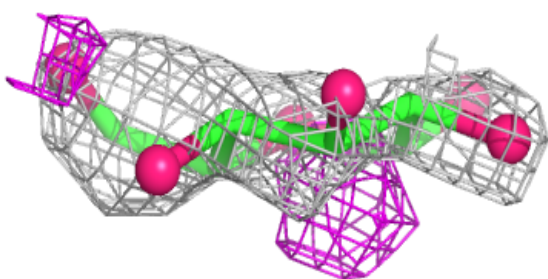
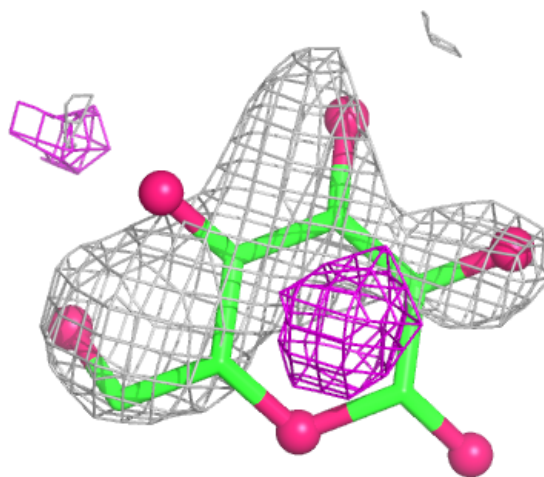
Electron density around BGC A 401:

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



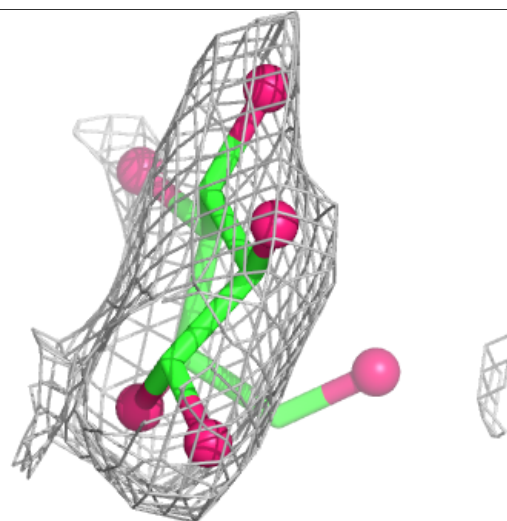
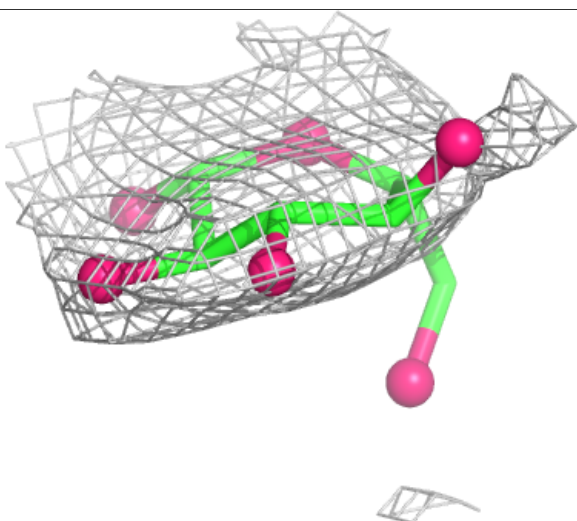
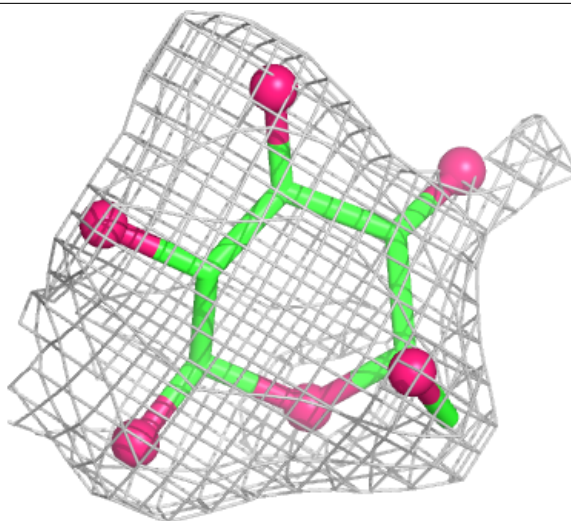
Electron density around BGC F 401:

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



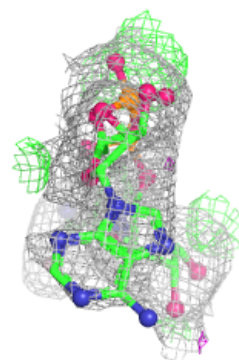
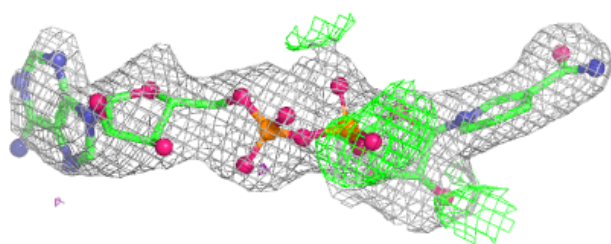
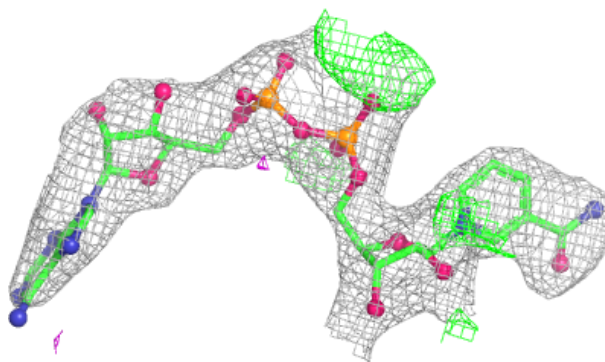
Electron density around BGC C 401:

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



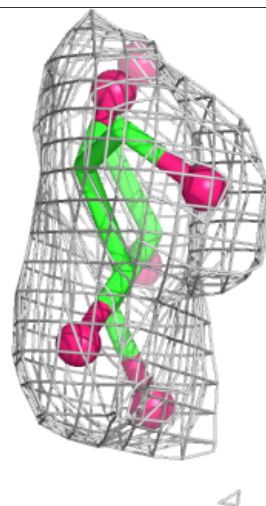
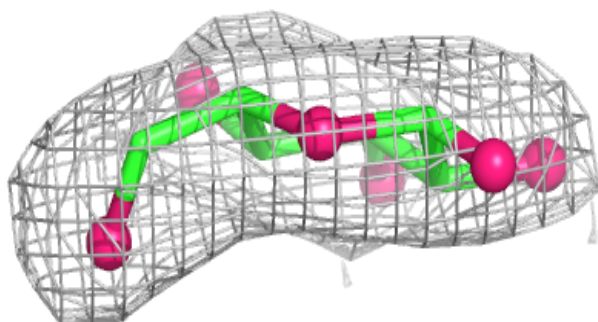
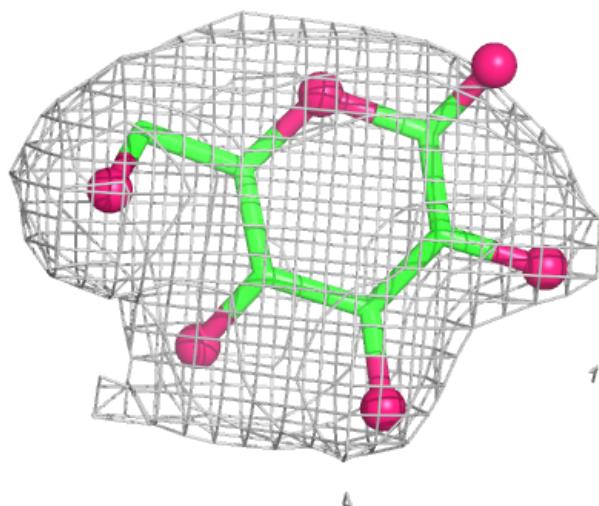
Electron density around NAD A 402:

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



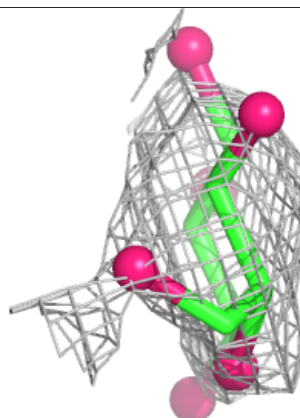
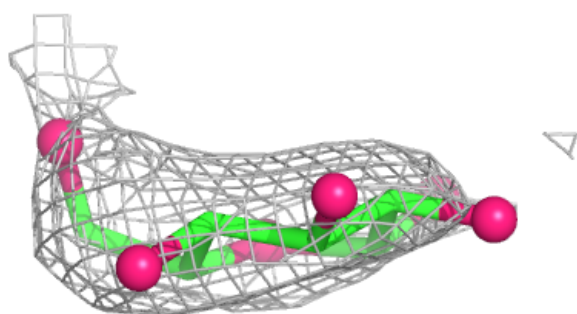
Electron density around BGC E 401:

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

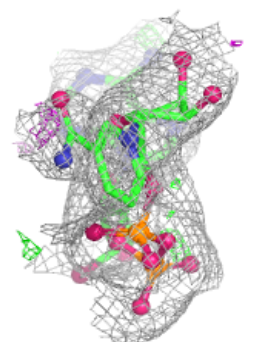
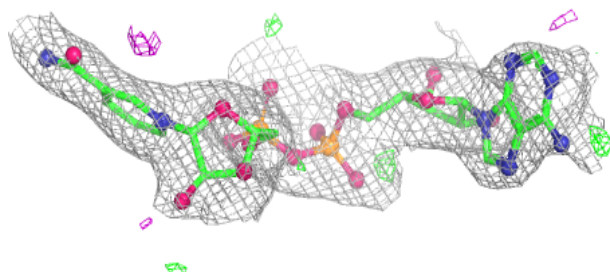
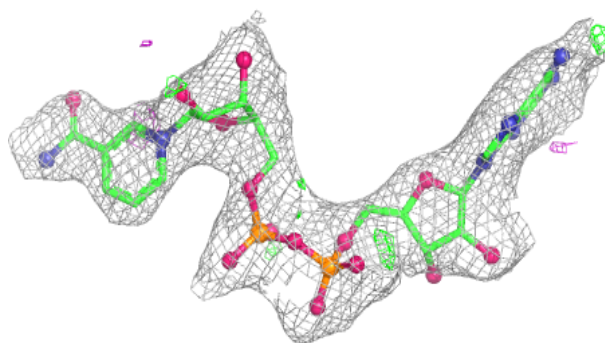


Electron density around BGC D 401:

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

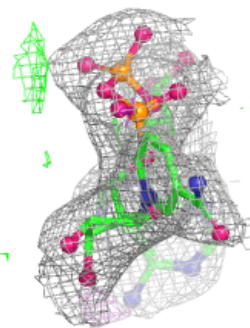
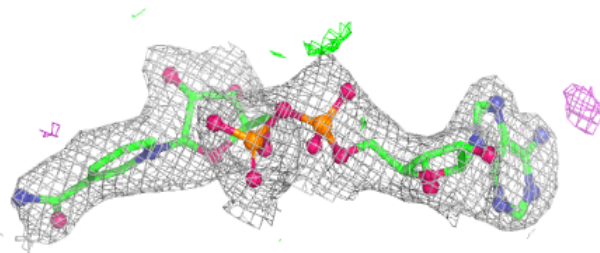
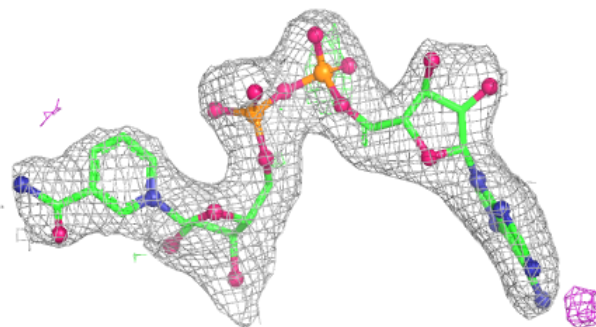
**Electron density around NAD D 402:**

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

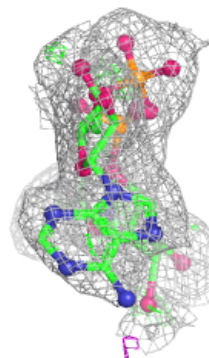
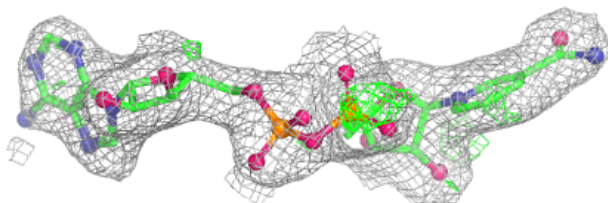
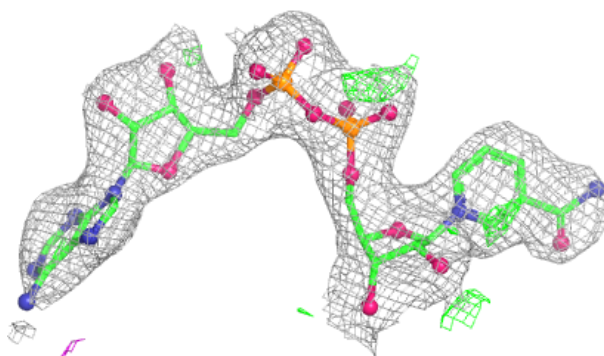


Electron density around NAD F 402:

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

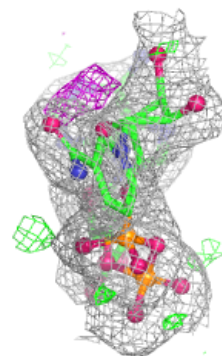
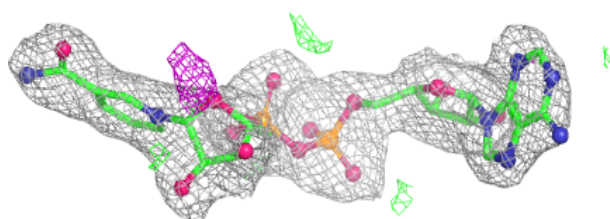
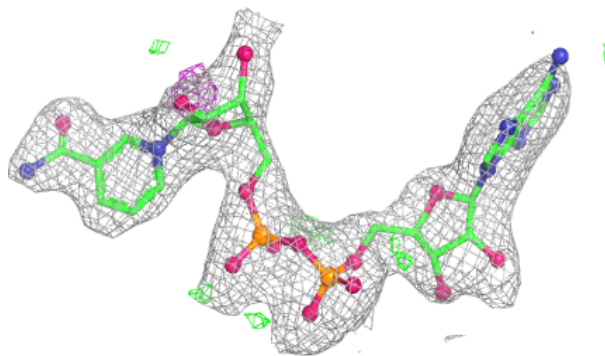
**Electron density around NAD E 402:**

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

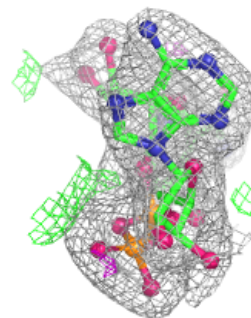
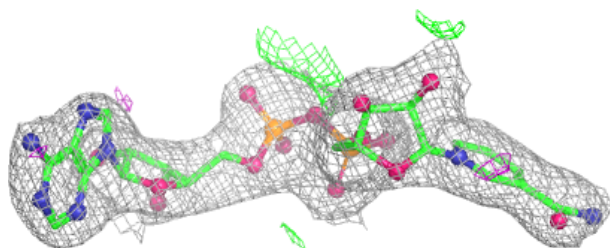
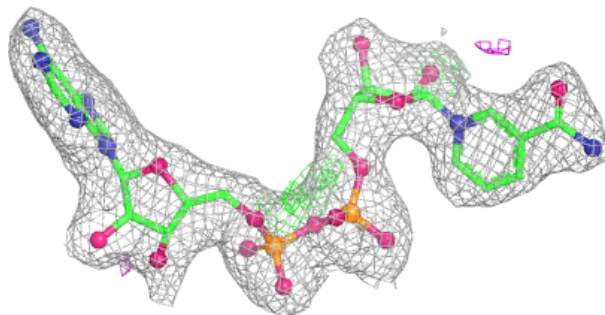


Electron density around NAD C 402:

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

**Electron density around NAD B 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.