



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:37 PM UTC

PDB ID : 8OHA / pdb_00008oha
Title : Crystal structure of Leptospira interrogans GAPDH
Authors : Navas-Yuste, S.; de la Paz, K.; Querol-Garcia, J.; Gomez-Quevedo, S.; Rodriguez de Cordoba, S.; Fernandez, F.J.; Vega, M.C.
Deposited on : 2023-03-20
Resolution : 2.37 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:

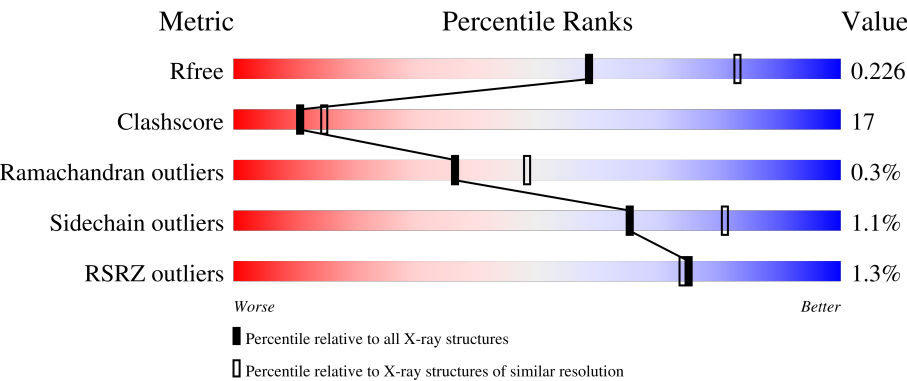
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.37 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.



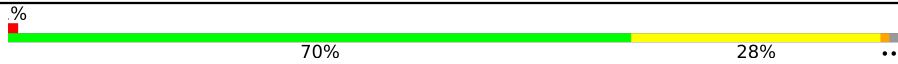
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	337	% 74% 25% ..
1	B	337	% 73% 26% .
1	C	337	% 69% 29% .
1	D	337	% 73% 25% ..
1	F	337	2% 71% 28% ..

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Mol	Chain	Length	Quality of chain
1	G	337	
1	H	337	
2	E	337	

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
3	PEG	B	402	-	-	X	-
4	GOL	B	409	-	-	X	-
4	GOL	D	405	-	-	X	-
4	GOL	D	408	-	-	X	-
4	GOL	H	403	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21537 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2566	1620	437	493	16			
1	B	336	Total	C	N	O	S	0	2	0
			2588	1632	440	500	16			
1	C	334	Total	C	N	O	S	0	0	0
			2566	1620	437	493	16			
1	D	333	Total	C	N	O	S	0	0	0
			2557	1614	435	492	16			
1	F	335	Total	C	N	O	S	0	0	0
			2571	1623	438	494	16			
1	G	334	Total	C	N	O	S	0	0	0
			2566	1620	437	493	16			
1	H	334	Total	C	N	O	S	0	0	0
			2562	1617	436	493	16			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q72QM3
A	0	ALA	-	expression tag	UNP Q72QM3
B	-1	GLY	-	expression tag	UNP Q72QM3
B	0	ALA	-	expression tag	UNP Q72QM3
C	-1	GLY	-	expression tag	UNP Q72QM3
C	0	ALA	-	expression tag	UNP Q72QM3
D	-1	GLY	-	expression tag	UNP Q72QM3
D	0	ALA	-	expression tag	UNP Q72QM3
F	-1	GLY	-	expression tag	UNP Q72QM3
F	0	ALA	-	expression tag	UNP Q72QM3
G	-1	GLY	-	expression tag	UNP Q72QM3
G	0	ALA	-	expression tag	UNP Q72QM3
H	-1	GLY	-	expression tag	UNP Q72QM3
H	0	ALA	-	expression tag	UNP Q72QM3

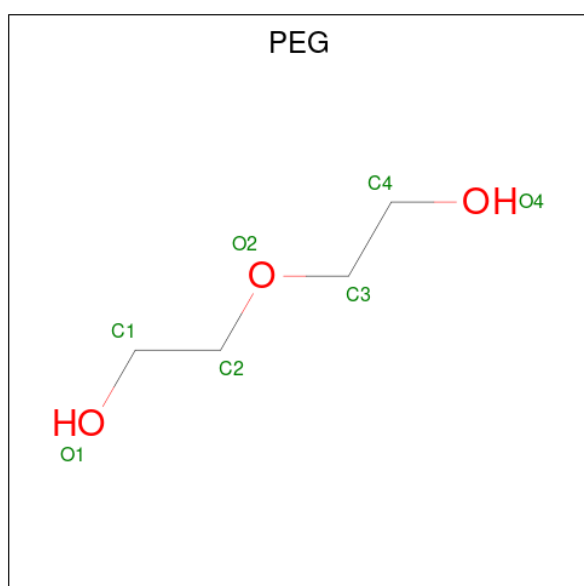
- Molecule 2 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	334	Total	C	N	O	S	0	0	0
			2564	1620	437	491	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP Q72QM3
E	0	ALA	-	expression tag	UNP Q72QM3

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



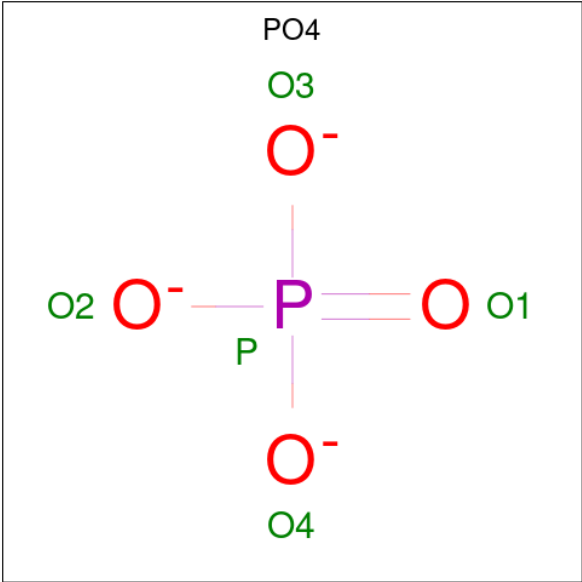
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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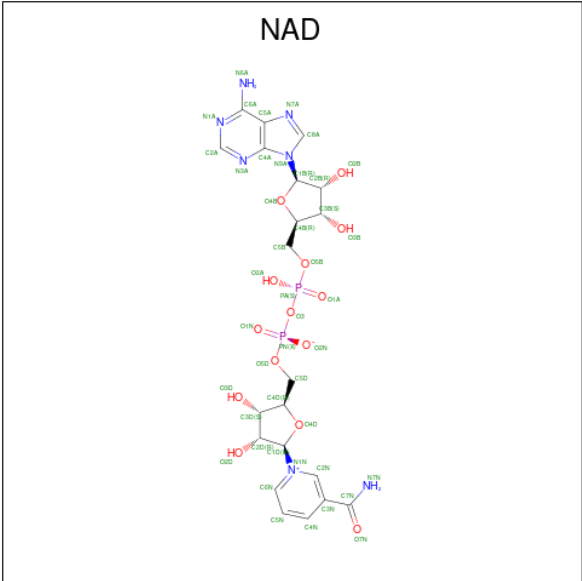
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

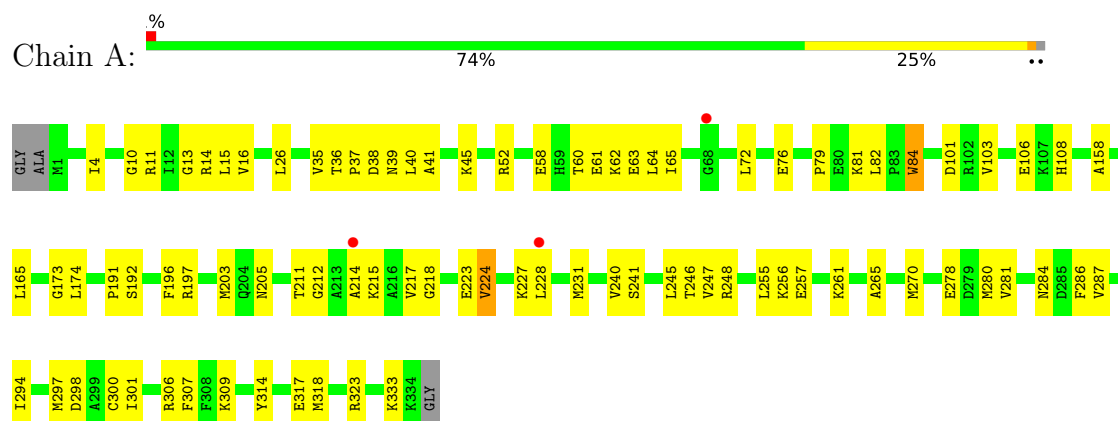
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	62	Total	O	0	0
			62	62		
7	B	71	Total	O	0	0
			71	71		
7	C	53	Total	O	0	0
			53	53		
7	D	54	Total	O	0	1
			55	55		
7	E	28	Total	O	0	0
			28	28		
7	F	29	Total	O	0	1
			30	30		
7	G	34	Total	O	0	0
			34	34		
7	H	45	Total	O	0	0
			45	45		

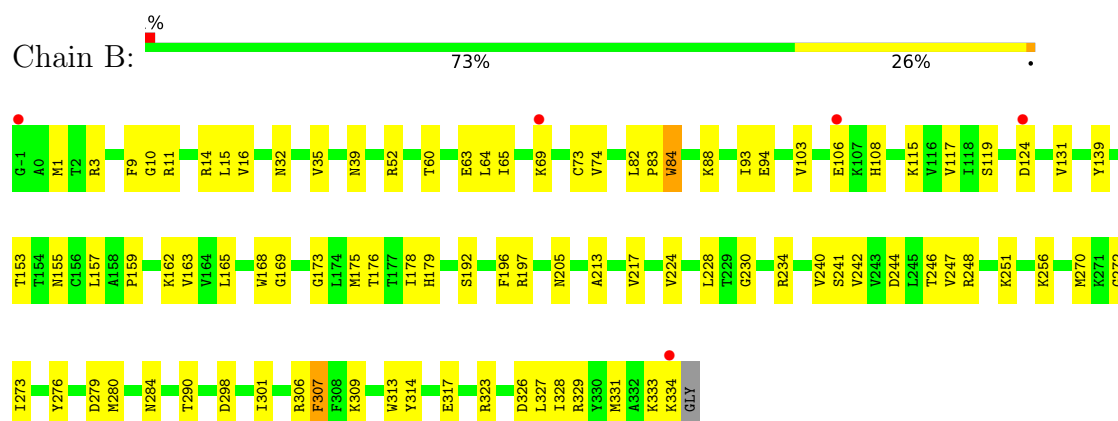
3 Residue-property plots

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.

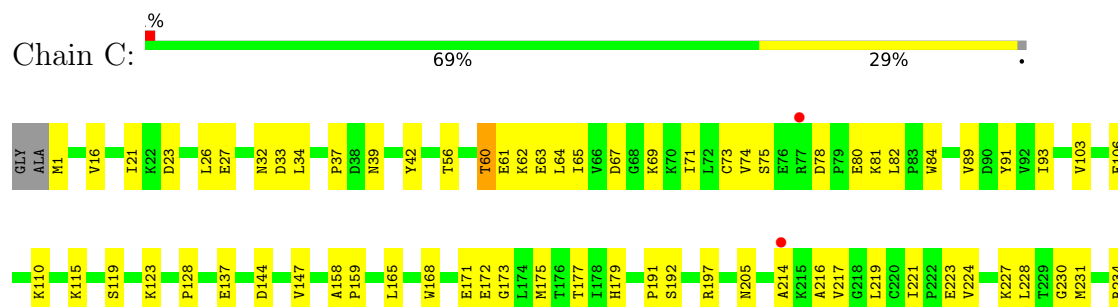
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

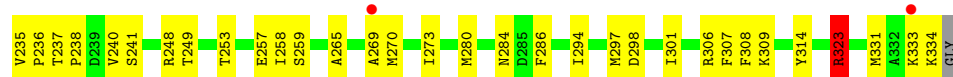


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

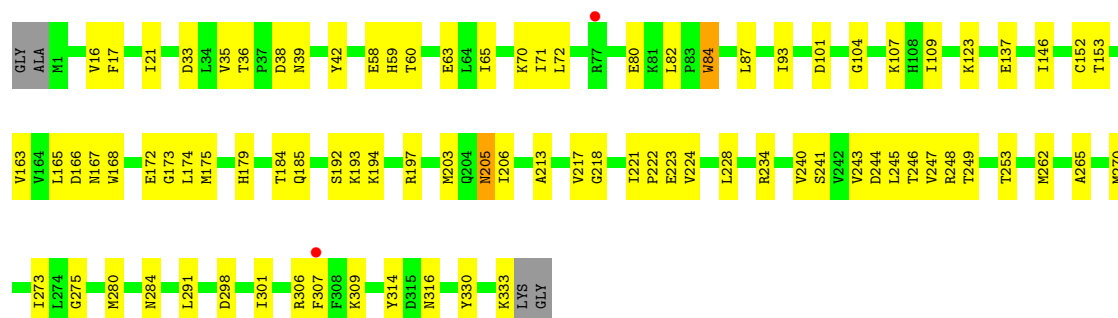
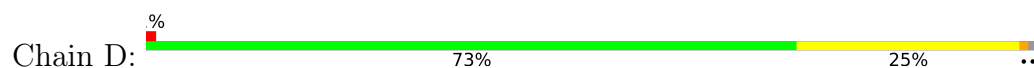


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

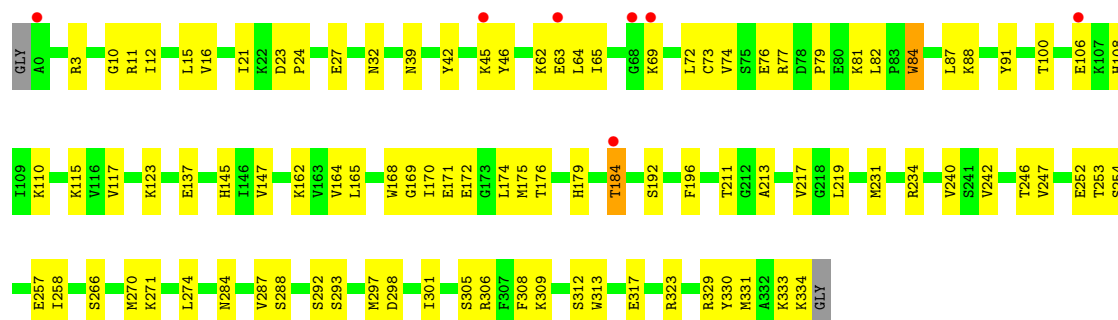




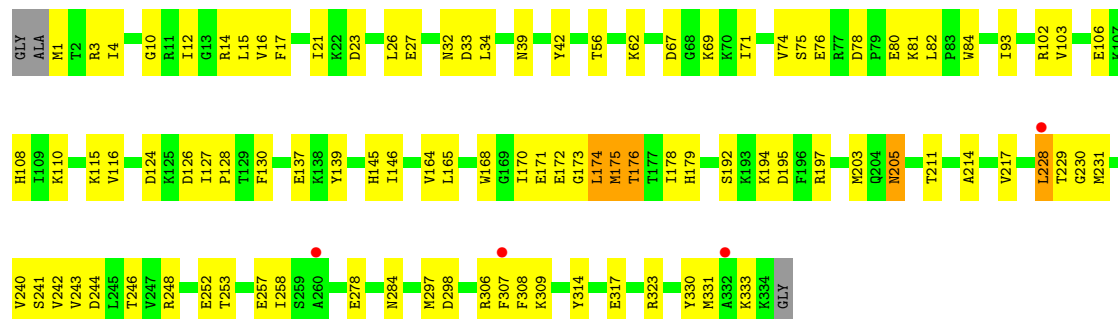
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

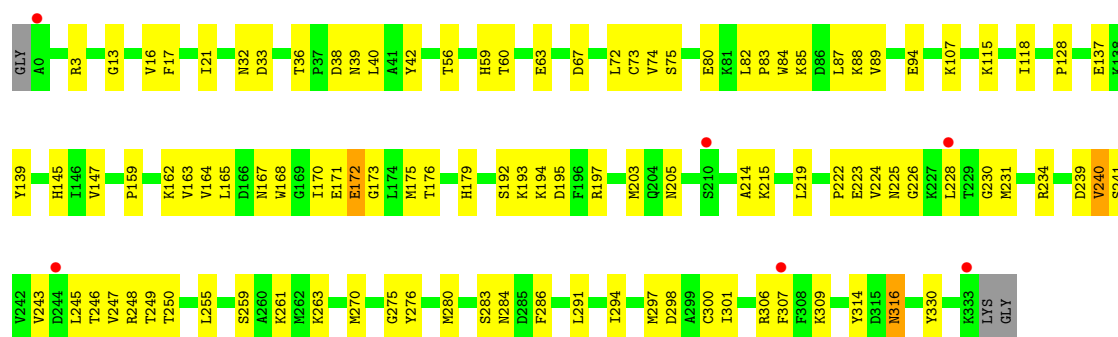


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

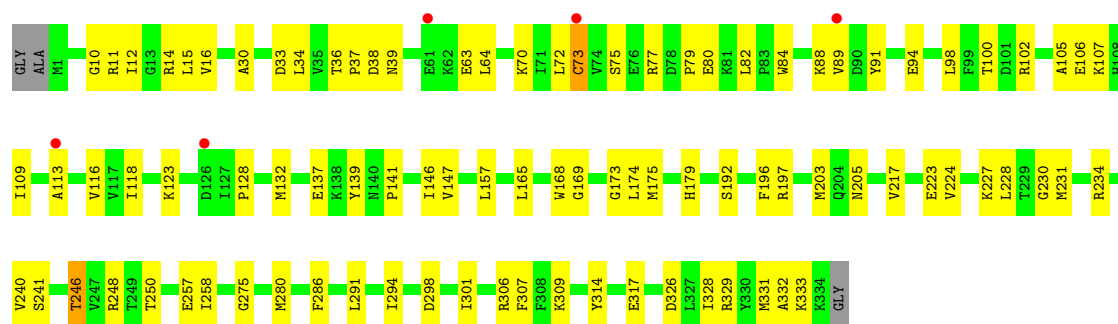


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase





• Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.80Å 82.04Å 123.18Å 94.02° 95.15° 112.52°	Depositor
Resolution (Å)	45.50 – 2.37 45.50 – 2.37	Depositor EDS
% Data completeness (in resolution range)	94.8 (45.50-2.37) 94.8 (45.50-2.37)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.21rc1_4903: ???)	Depositor
R, R_{free}	0.191 , 0.234 (Not available) , 0.226	Depositor DCC
R_{free} test set	2009 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21537	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.03% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, NAD, PEG, GOL, PO4

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	0.52	0/2602	0.72	0/3519
1	B	0.49	0/2627	0.71	0/3553
1	C	0.50	0/2602	0.70	0/3519
1	D	0.51	0/2593	0.73	2/3508 (0.1%)
1	F	0.52	0/2607	0.73	0/3526
1	G	0.62	2/2602 (0.1%)	0.85	5/3519 (0.1%)
1	H	0.50	1/2598 (0.0%)	0.67	0/3515
2	E	0.47	0/2608	0.67	0/3527
All	All	0.52	3/20839 (0.0%)	0.72	7/28186 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	F	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	174	LEU	C-N	10.35	1.47	1.33
1	H	83	PRO	CA-CB	9.90	1.59	1.53
1	G	175	MET	C-N	7.25	1.43	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	333	LYS	CD-CE-NZ	-8.17	85.76	111.90
1	G	174	LEU	O-C-N	6.73	131.31	123.30
1	D	205	ASN	N-CA-C	5.42	118.06	109.50
1	D	206	ILE	N-CA-C	-5.39	99.98	108.23
1	G	205	ASN	N-CA-C	5.27	117.69	109.52
1	G	174	LEU	CA-C-N	-5.14	115.48	122.93
1	G	174	LEU	C-N-CA	-5.14	115.48	122.93

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	323	ARG	Sidechain
1	F	77	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2566	0	2608	89	0
1	B	2588	0	2623	97	0
1	C	2566	0	2608	98	0
1	D	2557	0	2595	86	0
1	F	2571	0	2613	94	0
1	G	2566	0	2608	108	0
1	H	2562	0	2600	102	0
2	E	2564	0	2608	95	0
3	A	14	0	20	2	0
3	B	21	0	30	7	0
3	D	7	0	10	1	0
3	H	7	0	10	1	0
4	A	54	0	72	6	0
4	B	36	0	48	8	0
4	C	24	0	32	4	0
4	D	42	0	56	16	0
4	E	12	0	16	3	0
4	F	6	0	8	0	0
4	H	24	0	32	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	0	0
5	B	10	0	0	0	0
5	D	5	0	0	0	0
6	A	44	0	26	1	0
6	B	44	0	26	2	0
6	C	44	0	26	2	0
6	D	44	0	26	2	0
6	E	44	0	26	3	0
6	F	44	0	26	1	0
6	G	44	0	26	1	0
6	H	44	0	26	3	0
7	A	62	0	0	1	0
7	B	71	0	0	1	0
7	C	53	0	0	1	0
7	D	55	0	0	1	0
7	E	28	0	0	0	0
7	F	30	0	0	3	0
7	G	34	0	0	1	0
7	H	45	0	0	1	0
All	All	21537	0	21405	703	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 17.

All (703) 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)
2:E:309:LYS:HD3	1:F:231:MET:HE2	1.23	1.15
1:G:309:LYS:HD3	1:H:231:MET:HE2	1.32	1.12
1:F:63:GLU:HG2	1:F:72:LEU:HA	1.18	1.09
1:F:42:TYR:HA	1:F:45:LYS:HE2	1.37	1.04
1:A:280:MET:HE1	4:A:412:GOL:H2	1.44	1.00
1:B:39:ASN:HD21	1:C:192:SER:H	1.08	0.97
1:A:265:ALA:HB1	1:A:270:MET:HE2	1.43	0.97
1:A:192:SER:H	1:D:39:ASN:HD21	1.04	0.97
2:E:192:SER:H	1:H:39:ASN:HD21	1.06	0.96
1:A:39:ASN:HD21	1:D:192:SER:H	1.16	0.94
1:B:192:SER:H	1:C:39:ASN:HD21	1.15	0.93
2:E:39:ASN:HD21	1:H:192:SER:H	1.16	0.93
1:C:60:THR:HG22	1:C:62:LYS:H	1.30	0.91
1:C:159:PRO:HB3	1:C:270:MET:HE2	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:ASN:HD21	1:G:192:SER:H	1.12	0.90
1:A:63:GLU:HG2	1:A:72:LEU:HA	1.54	0.90
1:H:80:GLU:OE2	1:H:107:LYS:HG2	1.71	0.89
1:G:309:LYS:HD3	1:H:231:MET:CE	2.02	0.89
1:F:63:GLU:CG	1:F:72:LEU:HA	2.02	0.89
1:G:278:GLU:HG2	1:G:297:MET:HE3	1.52	0.88
1:C:273:ILE:HD13	1:C:323:ARG:HE	1.38	0.87
1:B:168:TRP:HA	1:B:251:LYS:HE3	1.55	0.86
1:D:175:MET:HE1	1:D:243:VAL:HG22	1.57	0.85
1:G:4:ILE:HD11	1:G:26:LEU:HD12	1.59	0.84
1:D:60:THR:OG1	1:D:63:GLU:HG2	1.76	0.83
1:F:82:LEU:HD13	1:F:84:TRP:CZ2	2.13	0.82
1:G:164:VAL:HG12	1:G:170:ILE:HD11	1.60	0.82
1:G:115:LYS:CD	1:G:145:HIS:HA	2.10	0.81
1:C:165:LEU:HD11	1:C:223:GLU:HB2	1.62	0.81
1:B:162:LYS:HD3	1:B:270:MET:CE	2.10	0.81
2:E:100:THR:OG1	2:E:123:LYS:HE3	1.79	0.81
1:C:228:LEU:HD12	1:C:228:LEU:O	1.81	0.80
1:C:249:THR:HG22	1:C:306:ARG:HA	1.62	0.80
1:D:58:GLU:HB2	1:D:65:ILE:HB	1.62	0.80
2:E:37:PRO:HG3	2:E:73:CYS:SG	2.21	0.80
1:A:318:MET:HA	1:A:318:MET:HE3	1.64	0.79
2:E:33:ASP:OD1	6:E:403:NAD:H1B	1.82	0.79
1:B:327:LEU:HG	1:B:331:MET:HE2	1.65	0.79
2:E:309:LYS:CD	1:F:231:MET:HE2	2.10	0.79
1:G:248:ARG:HD2	1:G:307:PHE:CZ	2.17	0.79
2:E:137:GLU:OE2	4:E:402:GOL:H2	1.83	0.78
1:A:60:THR:HG22	1:A:62:LYS:H	1.49	0.78
1:G:231:MET:HE3	1:H:309:LYS:HD3	1.66	0.77
2:E:34:LEU:HD21	2:E:77:ARG:HG2	1.66	0.77
1:C:1:MET:HE2	1:C:27:GLU:HB2	1.67	0.77
1:H:234:ARG:HH22	4:H:403:GOL:C1	1.98	0.77
1:B:52:ARG:HH12	3:B:403:PEG:H22	1.49	0.77
1:A:192:SER:H	1:D:39:ASN:ND2	1.82	0.76
1:B:328:ILE:HA	1:B:331:MET:HE3	1.67	0.76
1:C:159:PRO:HB3	1:C:270:MET:CE	2.15	0.76
1:F:63:GLU:HG2	1:F:72:LEU:CA	2.10	0.76
1:C:248:ARG:HD2	1:C:307:PHE:CZ	2.21	0.75
2:E:174:LEU:HD22	1:F:246:THR:HG23	1.69	0.75
1:D:38:ASP:HB2	4:D:408:GOL:H31	1.67	0.75
1:B:103:VAL:O	1:B:106:GLU:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:THR:HB	1:B:244[B]:ASP:OD1	1.87	0.74
1:C:78:ASP:HB3	1:C:81:LYS:HD2	1.69	0.74
2:E:63:GLU:OE2	2:E:70:LYS:HB3	1.86	0.74
1:H:228:LEU:HD12	1:H:228:LEU:O	1.88	0.74
1:D:163:VAL:HG21	1:D:262:MET:SD	2.28	0.73
1:H:263:LYS:HD3	1:H:276:TYR:CE2	2.23	0.73
1:F:192:SER:H	1:G:39:ASN:HD21	1.34	0.73
1:G:82:LEU:HD13	1:G:84:TRP:CZ2	2.23	0.73
1:H:214:ALA:O	1:H:228:LEU:HD11	1.87	0.73
1:F:21:ILE:HD11	1:F:69:LYS:HD2	1.70	0.73
1:G:23:ASP:HB3	1:G:26:LEU:HD23	1.71	0.72
1:D:123:LYS:HA	1:D:123:LYS:HE2	1.71	0.72
1:D:223:GLU:OE2	1:D:223:GLU:N	2.17	0.72
1:D:265:ALA:HB1	1:D:270:MET:CE	2.19	0.72
1:C:175:MET:HE3	1:C:230:GLY:HA3	1.72	0.71
2:E:192:SER:H	1:H:39:ASN:ND2	1.87	0.71
1:C:273:ILE:CD1	1:C:323:ARG:HE	2.04	0.70
1:F:253:THR:HA	1:F:257:GLU:OE1	1.92	0.70
2:E:248:ARG:HD2	2:E:307:PHE:CZ	2.26	0.70
2:E:329:ARG:O	2:E:333:LYS:HE2	1.92	0.70
1:A:103:VAL:O	1:A:106:GLU:HG2	1.91	0.70
1:B:290:THR:HG23	3:B:402:PEG:H22	1.72	0.70
1:F:137:GLU:OE2	1:F:137:GLU:N	2.22	0.70
1:G:17:PHE:CZ	1:G:21:ILE:HD13	2.26	0.70
1:D:59:HIS:NE2	4:D:408:GOL:H12	2.07	0.69
4:B:409:GOL:H32	4:D:408:GOL:H2	1.74	0.69
2:E:175:MET:HG3	2:E:230:GLY:HA3	1.75	0.69
1:C:23:ASP:OD2	1:C:26:LEU:HG	1.93	0.68
1:F:171:GLU:O	1:F:172:GLU:HG3	1.92	0.68
1:H:115:LYS:HE2	1:H:145:HIS:ND1	2.07	0.68
2:E:34:LEU:CD2	2:E:77:ARG:HG2	2.24	0.68
1:B:115:LYS:NZ	1:B:139:TYR:OH	2.25	0.68
1:C:269:ALA:O	1:C:270:MET:HB2	1.93	0.68
2:E:328:ILE:HA	2:E:331:MET:HE2	1.74	0.68
1:D:248:ARG:HD2	1:D:307:PHE:CZ	2.29	0.68
1:G:103:VAL:O	1:G:106:GLU:HG2	1.93	0.68
1:G:217:VAL:HG13	1:G:228:LEU:HD21	1.76	0.68
1:D:38:ASP:HB2	4:D:408:GOL:H11	1.76	0.68
1:B:39:ASN:ND2	1:C:192:SER:H	1.88	0.67
1:A:36:THR:HG22	1:A:37:PRO:HD2	1.75	0.67
1:F:91:TYR:HE1	1:F:331:MET:HE2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ALA:O	1:C:228:LEU:HD11	1.95	0.67
1:F:254:SER:OG	1:F:257:GLU:HG3	1.95	0.67
1:A:203:MET:HG2	1:D:203:MET:HG2	1.77	0.67
2:E:137:GLU:CD	4:E:402:GOL:H2	2.19	0.67
1:D:265:ALA:HB1	1:D:270:MET:HE3	1.77	0.67
1:G:76:GLU:HG2	1:G:81:LYS:HB2	1.77	0.67
2:E:91:TYR:CE1	2:E:331:MET:HE3	2.30	0.66
1:G:214:ALA:O	1:G:217:VAL:HG12	1.95	0.66
4:H:403:GOL:H32	6:H:406:NAD:C2N	2.26	0.66
2:E:223:GLU:OE2	2:E:223:GLU:N	2.22	0.66
1:B:60:THR:OG1	1:B:63:GLU:HG2	1.96	0.65
1:F:62:LYS:O	1:F:63:GLU:HG3	1.96	0.65
1:H:60:THR:OG1	1:H:63:GLU:HG2	1.96	0.65
1:B:251:LYS:CE	4:B:406:GOL:H11	2.27	0.65
1:D:82:LEU:HD13	1:D:84:TRP:CZ2	2.32	0.65
1:H:32:ASN:OD1	1:H:74:VAL:HG23	1.96	0.65
1:B:290:THR:H	3:B:402:PEG:H22	1.61	0.65
1:B:64:LEU:HD13	1:B:73:CYS:SG	2.36	0.65
1:B:248:ARG:HB2	1:B:307:PHE:CE1	2.32	0.65
1:B:157:LEU:HD22	1:B:175:MET:HE3	1.78	0.65
1:B:32:ASN:OD1	1:B:74:VAL:HG23	1.96	0.64
1:C:197:ARG:NH2	1:D:298:ASP:HB3	2.13	0.64
1:A:192:SER:N	1:D:39:ASN:HD21	1.87	0.64
1:G:197:ARG:NH2	1:H:298:ASP:HB3	2.13	0.64
1:F:45:LYS:HG3	1:F:46:TYR:CD2	2.31	0.64
1:A:280:MET:HE1	4:A:412:GOL:C2	2.24	0.64
1:B:251:LYS:HE2	4:B:406:GOL:H11	1.79	0.64
1:F:91:TYR:CE1	1:F:331:MET:HE2	2.31	0.64
1:F:106:GLU:OE2	1:F:110:LYS:HG3	1.98	0.64
1:F:165:LEU:HD12	1:F:169:GLY:HA2	1.79	0.64
1:H:249:THR:O	1:H:306:ARG:NE	2.30	0.64
1:A:36:THR:CG2	1:A:37:PRO:HD2	2.28	0.64
1:A:191:PRO:HB3	1:D:35:VAL:HG11	1.80	0.64
1:B:276:TYR:N	4:B:404:GOL:O3	2.27	0.64
1:A:173:GLY:C	1:A:174:LEU:HD12	2.23	0.63
1:B:52:ARG:HH22	3:B:403:PEG:H11	1.62	0.63
1:G:115:LYS:NZ	1:G:139:TYR:OH	2.31	0.63
1:G:309:LYS:HE2	1:H:176:THR:OG1	1.97	0.63
1:F:72:LEU:HD23	1:F:87:LEU:HD11	1.80	0.63
1:C:165:LEU:HD11	1:C:223:GLU:CB	2.28	0.63
1:C:249:THR:HG22	1:C:306:ARG:CA	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:SER:N	1:H:39:ASN:HD21	1.90	0.63
2:E:36:THR:HG23	1:H:193:LYS:HZ1	1.64	0.63
1:G:298:ASP:HB3	1:H:197:ARG:NH2	2.14	0.62
1:A:231:MET:HE3	3:A:401:PEG:H42	1.81	0.62
1:C:80:GLU:HG3	1:C:110:LYS:HD2	1.80	0.62
1:G:115:LYS:HE2	1:G:145:HIS:ND1	2.14	0.62
1:C:237:THR:HG23	1:C:238:PRO:HD2	1.82	0.62
1:G:110:LYS:HD3	1:G:110:LYS:C	2.25	0.62
1:G:164:VAL:HG12	1:G:170:ILE:CD1	2.29	0.62
2:E:196:PHE:HB3	1:H:42:TYR:CE2	2.34	0.62
1:D:221:ILE:O	1:D:224:VAL:HG22	2.01	0.61
1:F:162:LYS:HD3	1:F:270:MET:CE	2.30	0.61
1:F:252:GLU:HB3	1:F:305:SER:OG	2.01	0.61
1:H:214:ALA:HB1	1:H:228:LEU:HD13	1.80	0.61
1:B:82:LEU:HD13	1:B:84:TRP:CZ2	2.34	0.61
1:G:110:LYS:HD3	1:G:110:LYS:O	2.00	0.61
1:D:38:ASP:HB2	4:D:408:GOL:C3	2.30	0.61
1:F:39:ASN:ND2	1:G:192:SER:H	1.93	0.61
1:G:76:GLU:CG	1:G:81:LYS:HB2	2.31	0.61
1:C:165:LEU:CD1	1:C:223:GLU:HB2	2.29	0.61
1:C:249:THR:CG2	1:C:306:ARG:HA	2.31	0.61
1:F:266:SER:HB2	1:F:274:LEU:O	2.00	0.61
4:A:404:GOL:H31	4:A:406:GOL:H11	1.82	0.61
1:G:76:GLU:OE2	1:G:81:LYS:HD2	2.00	0.61
1:A:36:THR:HB	1:A:38:ASP:OD1	2.01	0.60
1:G:115:LYS:HD3	1:G:145:HIS:HA	1.83	0.60
1:C:103:VAL:O	1:C:106:GLU:HG2	2.01	0.60
1:D:245:LEU:HG	1:D:247:VAL:HG22	1.83	0.60
2:E:39:ASN:ND2	1:H:192:SER:H	1.93	0.60
1:G:21:ILE:CD1	1:G:69:LYS:HE2	2.32	0.60
1:A:60:THR:CG2	1:A:61:GLU:N	2.64	0.60
1:B:248:ARG:HB2	1:B:307:PHE:HE1	1.64	0.60
1:C:56:THR:HG22	1:C:67:ASP:HA	1.82	0.60
1:F:171:GLU:C	1:F:172:GLU:HG3	2.25	0.60
1:G:252:GLU:HG2	1:G:306:ARG:HG3	1.83	0.60
1:H:173:GLY:O	1:H:228:LEU:HA	2.00	0.60
2:E:157:LEU:HD22	2:E:175:MET:HE3	1.82	0.60
1:F:79:PRO:HB3	1:F:108:HIS:CE1	2.36	0.60
1:F:106:GLU:OE1	1:F:110:LYS:HE3	2.01	0.60
1:C:234:ARG:HH21	4:C:402:GOL:C1	2.14	0.60
1:A:245:LEU:HG	1:A:247:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:MET:HE2	1:D:243:VAL:HG13	1.84	0.60
1:C:265:ALA:O	1:C:269:ALA:O	2.20	0.60
1:A:265:ALA:HB1	1:A:270:MET:CE	2.28	0.60
1:H:234:ARG:HH22	4:H:403:GOL:H11	1.66	0.59
1:G:197:ARG:HH21	1:H:298:ASP:HB3	1.66	0.59
1:G:16:VAL:HG11	1:G:93:ILE:HD13	1.83	0.59
1:A:60:THR:HG22	1:A:61:GLU:N	2.17	0.59
1:F:15:LEU:CD1	1:F:317:GLU:HB3	2.33	0.59
1:B:153:THR:CG2	1:B:175:MET:HE1	2.33	0.59
1:H:171:GLU:HB3	1:H:172:GLU:OE1	2.03	0.59
1:G:139:TYR:CE1	1:G:331:MET:HE3	2.36	0.59
1:G:175:MET:HE1	1:G:211:THR:HG21	1.85	0.59
1:H:175:MET:HE1	1:H:243:VAL:HG22	1.85	0.59
1:B:52:ARG:NH2	3:B:403:PEG:H11	2.17	0.59
1:G:278:GLU:HG2	1:G:297:MET:CE	2.30	0.59
2:E:84:TRP:HE3	2:E:84:TRP:HA	1.69	0.58
1:H:194:LYS:HG3	1:H:195:ASP:N	2.16	0.58
1:A:39:ASN:ND2	1:D:192:SER:H	1.94	0.58
2:E:137:GLU:OE1	4:E:402:GOL:H32	2.03	0.58
1:G:253:THR:HG23	1:G:308:PHE:CZ	2.38	0.58
1:C:234:ARG:HH21	4:C:402:GOL:H11	1.69	0.58
1:F:252:GLU:HG3	1:F:306:ARG:HH11	1.68	0.58
1:G:309:LYS:CD	1:H:231:MET:HE2	2.21	0.58
1:A:174:LEU:HD23	1:B:309:LYS:HB2	1.86	0.58
1:F:213:ALA:O	1:F:217:VAL:HG23	2.03	0.58
1:G:165:LEU:HA	1:G:170:ILE:HD12	1.85	0.57
1:A:246:THR:HG23	7:A:532:HOH:O	2.04	0.57
1:A:280:MET:HE3	1:B:197:ARG:HG3	1.85	0.57
2:E:231:MET:HB3	1:F:301:ILE:HD13	1.86	0.57
1:A:278:GLU:HG2	1:A:297:MET:CE	2.34	0.57
1:B:224:VAL:HG11	1:B:228:LEU:HD11	1.86	0.57
1:D:59:HIS:CD2	4:D:408:GOL:H12	2.40	0.57
2:E:241:SER:HB2	2:E:314:TYR:CZ	2.39	0.57
1:G:244:ASP:OD1	1:G:309:LYS:HE3	2.04	0.57
1:H:225:ASN:OD1	1:H:226:GLY:N	2.38	0.57
2:E:84:TRP:HA	2:E:84:TRP:CE3	2.38	0.57
1:H:164:VAL:HG13	1:H:170:ILE:HD11	1.85	0.57
2:E:165:LEU:HD12	2:E:169:GLY:HA2	1.87	0.57
1:F:106:GLU:CD	1:F:110:LYS:HE3	2.30	0.57
1:C:32:ASN:OD1	1:C:74:VAL:HG23	2.05	0.57
1:D:234:ARG:HH22	4:D:405:GOL:H31	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ILE:HD13	1:B:323:ARG:NE	2.20	0.57
1:A:101:ASP:OD1	1:A:103:VAL:HG23	2.05	0.56
1:C:21:ILE:HD12	1:C:69:LYS:NZ	2.19	0.56
1:G:253:THR:HA	1:G:257:GLU:OE1	2.05	0.56
1:H:175:MET:HG3	1:H:230:GLY:HA3	1.86	0.56
1:F:32:ASN:OD1	1:F:74:VAL:HG23	2.05	0.56
1:A:245:LEU:HG	1:A:247:VAL:CG2	2.35	0.56
1:D:330:TYR:HA	1:D:333:LYS:HE3	1.88	0.56
1:F:301:ILE:HD11	1:F:309:LYS:HD2	1.88	0.56
2:E:275:GLY:HA3	2:E:291:LEU:HD13	1.87	0.56
1:H:72:LEU:HD13	1:H:73:CYS:N	2.21	0.56
1:C:91:TYR:HE2	1:C:331:MET:HE2	1.71	0.56
2:E:84:TRP:CE3	2:E:89:VAL:HG21	2.40	0.55
1:H:159:PRO:O	1:H:163:VAL:HG23	2.06	0.55
1:A:4:ILE:HD11	1:A:26:LEU:HD22	1.87	0.55
2:E:15:LEU:CD1	2:E:317:GLU:HB3	2.36	0.55
1:H:84:TRP:CE3	1:H:89:VAL:HG21	2.41	0.55
1:A:62:LYS:C	1:A:63:GLU:HG3	2.32	0.55
1:D:275:GLY:HA3	1:D:291:LEU:HD13	1.88	0.55
1:G:179:HIS:HA	1:G:241:SER:HB3	1.88	0.55
1:G:102:ARG:NH2	7:G:502:HOH:O	2.39	0.55
1:G:197:ARG:HG3	1:H:280:MET:HB3	1.88	0.55
1:A:278:GLU:HG2	1:A:297:MET:HE3	1.89	0.55
1:B:224:VAL:HG13	1:B:228:LEU:HG	1.89	0.54
1:D:185:GLN:OE1	1:D:234:ARG:NH1	2.38	0.54
1:G:205:ASN:OD1	1:H:284:ASN:HB2	2.07	0.54
1:B:84:TRP:HA	1:B:84:TRP:HE3	1.73	0.54
1:A:174:LEU:HD12	1:A:174:LEU:N	2.21	0.54
2:E:168:TRP:CH2	2:E:258:ILE:HA	2.42	0.54
1:H:234:ARG:HH22	4:H:403:GOL:H12	1.70	0.54
1:F:137:GLU:H	1:F:137:GLU:CD	2.14	0.54
1:G:127:ILE:HD13	1:G:146:ILE:HG22	1.89	0.54
1:G:173:GLY:HA2	1:G:246:THR:O	2.07	0.54
1:A:173:GLY:O	1:A:228:LEU:HA	2.06	0.54
2:E:102:ARG:O	2:E:106:GLU:HG2	2.07	0.54
1:F:65:ILE:HA	1:F:69:LYS:O	2.08	0.54
1:B:241:SER:HB2	1:B:314:TYR:CZ	2.43	0.54
1:D:249:THR:O	1:D:306:ARG:NH2	2.36	0.54
1:C:110:LYS:C	1:C:110:LYS:HD3	2.32	0.54
1:B:64:LEU:C	1:B:65:ILE:HD12	2.32	0.54
2:E:63:GLU:HA	2:E:73:CYS:SG	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:248:ARG:HD3	1:H:307:PHE:CZ	2.43	0.54
1:B:84:TRP:HA	1:B:84:TRP:CE3	2.43	0.54
1:D:33:ASP:OD1	6:D:410:NAD:O2B	2.22	0.54
1:G:231:MET:HE3	1:H:309:LYS:CD	2.35	0.54
1:A:62:LYS:O	1:A:63:GLU:HG3	2.08	0.53
1:H:84:TRP:HE3	1:H:84:TRP:HA	1.73	0.53
1:H:115:LYS:NZ	1:H:139:TYR:OH	2.40	0.53
1:G:284:ASN:HB2	1:H:205:ASN:OD1	2.08	0.53
1:C:159:PRO:HA	1:C:270:MET:HE1	1.90	0.53
1:F:253:THR:CA	1:F:257:GLU:OE1	2.56	0.53
1:G:172:GLU:OE1	1:G:248:ARG:HD3	2.08	0.53
1:C:60:THR:HG21	7:F:523:HOH:O	2.08	0.53
1:H:3:ARG:HH11	1:H:88:LYS:HB2	1.73	0.53
1:H:214:ALA:O	1:H:228:LEU:CD1	2.54	0.53
1:C:60:THR:CG2	1:C:61:GLU:N	2.71	0.53
1:A:165:LEU:HD21	1:A:223:GLU:HB2	1.91	0.53
1:C:119:SER:O	6:C:405:NAD:H1D	2.08	0.53
1:F:21:ILE:HD11	1:F:69:LYS:CD	2.38	0.53
1:F:175:MET:HE1	1:F:211:THR:HG21	1.91	0.53
1:G:84:TRP:HA	1:G:84:TRP:CE3	2.44	0.53
1:H:286:PHE:CD1	1:H:294:ILE:HD13	2.44	0.53
1:D:167:ASN:HB2	1:D:168:TRP:CE3	2.44	0.53
1:D:213:ALA:O	1:D:217:VAL:HG23	2.08	0.53
1:A:197:ARG:NH2	1:B:298:ASP:HB3	2.23	0.53
2:E:36:THR:HG23	1:H:193:LYS:NZ	2.22	0.53
1:B:159:PRO:O	1:B:163:VAL:HG23	2.09	0.52
1:C:221:ILE:O	1:C:224:VAL:HG22	2.08	0.52
2:E:10:GLY:HA3	6:E:403:NAD:O5B	2.08	0.52
2:E:228:LEU:O	2:E:228:LEU:HD12	2.09	0.52
2:E:329:ARG:O	2:E:333:LYS:CE	2.57	0.52
1:F:184:THR:HG23	7:F:526:HOH:O	2.07	0.52
1:D:17:PHE:CZ	1:D:71:ILE:HD13	2.44	0.52
2:E:34:LEU:CD2	2:E:77:ARG:CG	2.87	0.52
2:E:82:LEU:HD13	2:E:84:TRP:CZ2	2.44	0.52
1:G:323:ARG:HA	1:G:323:ARG:NE	2.24	0.52
1:A:301:ILE:HG12	1:A:309:LYS:HB3	1.92	0.52
1:D:193:LYS:HG3	1:D:194:LYS:HG2	1.91	0.52
1:D:245:LEU:HG	1:D:247:VAL:CG2	2.39	0.52
1:F:15:LEU:HD12	1:F:317:GLU:HB3	1.92	0.52
1:G:165:LEU:HB2	1:G:170:ILE:HD13	1.91	0.52
1:H:84:TRP:CE3	1:H:84:TRP:HA	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:GLU:CD	1:H:248:ARG:HE	2.18	0.52
1:B:15:LEU:CD1	1:B:317:GLU:HB3	2.39	0.52
1:C:168:TRP:HZ2	1:C:257:GLU:HG2	1.75	0.52
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.45	0.52
1:B:328:ILE:HA	1:B:331:MET:CE	2.39	0.52
1:D:38:ASP:CB	4:D:408:GOL:H11	2.40	0.52
1:G:78:ASP:OD2	1:G:80:GLU:CG	2.58	0.52
2:E:91:TYR:OH	2:E:332:ALA:HA	2.09	0.52
2:E:332:ALA:HB3	2:E:333:LYS:NZ	2.25	0.52
1:G:307:PHE:CE1	1:H:172:GLU:OE2	2.62	0.52
1:H:249:THR:O	1:H:306:ARG:NH2	2.42	0.52
1:A:214:ALA:O	1:A:217:VAL:HB	2.10	0.52
1:B:65:ILE:HD12	1:B:65:ILE:N	2.25	0.52
1:F:115:LYS:HD3	1:F:145:HIS:HA	1.91	0.52
1:G:32:ASN:OD1	1:G:74:VAL:HG23	2.10	0.52
1:B:280:MET:H	4:B:409:GOL:H2	1.75	0.52
1:C:84:TRP:HE3	1:C:84:TRP:HA	1.75	0.52
1:C:173:GLY:O	1:C:228:LEU:HA	2.10	0.52
2:E:100:THR:OG1	2:E:123:LYS:HG3	2.10	0.52
2:E:105:ALA:HB1	2:E:116:VAL:HG11	1.92	0.52
1:G:84:TRP:HA	1:G:84:TRP:HE3	1.74	0.52
1:C:259:SER:OG	1:C:297:MET:HG3	2.09	0.52
1:B:3:ARG:HD3	1:B:88:LYS:O	2.09	0.51
1:C:309:LYS:HE2	1:D:174:LEU:HB3	1.91	0.51
1:F:12:ILE:O	1:F:16:VAL:HG13	2.09	0.51
1:B:280:MET:HE1	1:B:298:ASP:CG	2.36	0.51
2:E:286:PHE:CE1	2:E:294:ILE:HG21	2.45	0.51
1:A:35:VAL:HG23	1:A:40:LEU:HD21	1.92	0.51
1:B:279:ASP:HA	4:B:409:GOL:O2	2.10	0.51
1:C:84:TRP:HA	1:C:84:TRP:CE3	2.45	0.51
1:C:197:ARG:HH21	1:D:298:ASP:HB3	1.75	0.51
1:F:100:THR:OG1	1:F:123:LYS:HG3	2.10	0.51
1:H:82:LEU:HD13	1:H:84:TRP:CZ2	2.46	0.51
1:A:286:PHE:CE1	1:A:294:ILE:HG21	2.46	0.51
1:C:64:LEU:HG	1:C:73:CYS:SG	2.51	0.51
2:E:333:LYS:HD3	2:E:333:LYS:N	2.26	0.51
1:G:175:MET:HG2	1:G:176:THR:N	2.26	0.51
1:H:179:HIS:HB3	1:H:234:ARG:HD3	1.92	0.51
1:H:245:LEU:HG	1:H:247:VAL:CG2	2.40	0.51
1:B:242:VAL:HB	1:B:313:TRP:CE3	2.45	0.51
1:C:228:LEU:HD12	1:C:228:LEU:C	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:HIS:HB3	1:F:234:ARG:HD3	1.92	0.51
1:G:178:ILE:HB	1:G:242:VAL:HG12	1.92	0.51
1:G:137:GLU:HA	1:G:330:TYR:OH	2.11	0.51
1:C:253:THR:HG23	1:C:308:PHE:CZ	2.46	0.50
1:B:15:LEU:HD12	1:B:317:GLU:HB3	1.93	0.50
1:C:21:ILE:HD11	1:C:69:LYS:HD3	1.92	0.50
1:C:16:VAL:HG11	1:C:93:ILE:HD13	1.92	0.50
1:D:72:LEU:HD23	1:D:87:LEU:HD11	1.93	0.50
1:G:243:VAL:HG23	1:G:314:TYR:CE1	2.46	0.50
1:G:278:GLU:CG	1:G:297:MET:HE3	2.34	0.50
1:B:224:VAL:HG11	1:B:228:LEU:CD1	2.40	0.50
1:C:33:ASP:OD1	1:C:34:LEU:N	2.42	0.50
1:D:84:TRP:CE3	1:D:84:TRP:HA	2.47	0.50
1:H:59:HIS:NE2	3:H:401:PEG:H42	2.26	0.50
1:A:76:GLU:HG2	1:A:81:LYS:HB2	1.93	0.50
1:F:242:VAL:HB	1:F:313:TRP:CE3	2.46	0.50
1:A:248:ARG:HD3	1:A:307:PHE:CZ	2.47	0.50
1:B:280:MET:HE1	1:B:298:ASP:OD1	2.12	0.50
1:F:84:TRP:HA	1:F:84:TRP:CE3	2.46	0.50
1:G:244:ASP:CG	1:G:309:LYS:HE3	2.36	0.50
1:D:234:ARG:NH2	4:D:405:GOL:H31	2.26	0.50
1:F:100:THR:OG1	1:F:123:LYS:HE3	2.12	0.50
1:D:244:ASP:OD1	1:D:309:LYS:HG2	2.12	0.49
1:B:192:SER:H	1:C:39:ASN:ND2	1.97	0.49
1:D:168:TRP:CD1	1:D:253:THR:HB	2.48	0.49
1:F:10:GLY:HA3	6:F:402:NAD:O5B	2.11	0.49
1:G:4:ILE:CD1	1:G:26:LEU:HD12	2.36	0.49
1:G:124:ASP:HB3	1:G:126:ASP:OD1	2.12	0.49
1:G:214:ALA:HA	1:G:228:LEU:HD11	1.94	0.49
1:B:246:THR:OG1	1:B:309:LYS:NZ	2.46	0.49
2:E:241:SER:HB2	2:E:314:TYR:CE1	2.47	0.49
1:D:38:ASP:CA	4:D:408:GOL:H11	2.42	0.49
2:E:84:TRP:O	2:E:88:LYS:N	2.45	0.49
1:A:248:ARG:CD	1:A:307:PHE:CZ	2.95	0.49
1:B:251:LYS:NZ	4:B:406:GOL:O2	2.46	0.49
2:E:64:LEU:N	2:E:64:LEU:HD12	2.28	0.49
1:H:33:ASP:OD2	6:H:406:NAD:O3B	2.25	0.49
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.48	0.49
1:C:298:ASP:HB3	1:D:197:ARG:NH2	2.27	0.49
1:H:167:ASN:HB2	1:H:168:TRP:CE3	2.48	0.49
1:A:197:ARG:HG3	1:B:280:MET:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ALA:O	1:B:217:VAL:HG23	2.13	0.49
1:C:56:THR:HG23	7:C:512:HOH:O	2.13	0.49
1:C:159:PRO:CA	1:C:270:MET:HE1	2.43	0.49
1:F:253:THR:HG23	1:F:308:PHE:CZ	2.48	0.49
1:H:72:LEU:HD12	1:H:74:VAL:HG13	1.95	0.49
1:C:214:ALA:O	1:C:217:VAL:CG1	2.62	0.48
2:E:174:LEU:HB3	1:F:309:LYS:HE2	1.95	0.48
1:F:106:GLU:OE1	1:F:106:GLU:C	2.56	0.48
1:F:333:LYS:O	1:F:334:LYS:HB2	2.12	0.48
1:A:298:ASP:OD1	4:A:412:GOL:H32	2.12	0.48
1:C:205:ASN:OD1	1:D:284:ASN:HB2	2.13	0.48
1:D:165:LEU:HD11	1:D:223:GLU:HB2	1.96	0.48
1:D:301:ILE:HG12	1:D:309:LYS:HB3	1.94	0.48
4:B:409:GOL:C3	4:D:408:GOL:H2	2.44	0.48
1:F:63:GLU:OE2	1:F:72:LEU:HD13	2.14	0.48
1:A:79:PRO:HB3	1:A:108:HIS:CE1	2.49	0.48
1:F:252:GLU:HG3	1:F:306:ARG:NH1	2.28	0.48
1:H:250:THR:HA	1:H:306:ARG:NH2	2.29	0.48
1:B:179:HIS:HB3	1:B:234:ARG:HD3	1.96	0.48
1:C:241:SER:HB2	1:C:314:TYR:CZ	2.49	0.48
1:H:33:ASP:O	1:H:75:SER:HA	2.13	0.48
1:B:323:ARG:HA	1:B:323:ARG:HD3	1.63	0.48
1:D:16:VAL:HG11	1:D:93:ILE:HD13	1.95	0.48
1:D:280:MET:HE1	4:D:401:GOL:H12	1.96	0.48
1:A:278:GLU:CD	1:A:297:MET:HE2	2.39	0.48
1:H:164:VAL:HG13	1:H:165:LEU:N	2.29	0.48
1:C:159:PRO:CB	1:C:270:MET:CE	2.90	0.48
1:D:175:MET:CE	1:D:243:VAL:HG22	2.38	0.48
1:G:12:ILE:O	1:G:16:VAL:HG23	2.13	0.48
1:C:84:TRP:CE3	1:C:89:VAL:HG21	2.49	0.48
1:D:137:GLU:HA	1:D:330:TYR:OH	2.14	0.48
1:F:117:VAL:HG22	1:F:147:VAL:CG2	2.44	0.48
1:G:21:ILE:HD12	1:G:69:LYS:HE2	1.95	0.48
1:G:33:ASP:OD1	1:G:34:LEU:N	2.41	0.48
1:H:228:LEU:HD12	1:H:228:LEU:C	2.38	0.48
1:B:196:PHE:HB3	1:C:42:TYR:CE2	2.48	0.47
1:C:128:PRO:HG2	1:C:147:VAL:HG12	1.95	0.47
1:D:17:PHE:CZ	1:D:21:ILE:HD12	2.49	0.47
2:E:309:LYS:HE2	1:F:176:THR:OG1	2.13	0.47
2:E:173:GLY:C	2:E:174:LEU:HD12	2.39	0.47
1:G:168:TRP:CH2	1:G:258:ILE:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248:ARG:CD	1:G:307:PHE:CZ	2.93	0.47
1:H:162:LYS:HD3	1:H:270:MET:CE	2.43	0.47
1:B:119:SER:O	6:B:412:NAD:H1D	2.14	0.47
1:D:301:ILE:HD11	1:D:309:LYS:HD2	1.97	0.47
2:E:196:PHE:HB3	1:H:42:TYR:CD2	2.49	0.47
1:F:84:TRP:HA	1:F:84:TRP:HE3	1.79	0.47
1:G:298:ASP:HB3	1:H:197:ARG:HH21	1.77	0.47
1:A:52:ARG:HH12	4:C:404:GOL:H12	1.79	0.47
1:G:115:LYS:HD2	1:G:145:HIS:HA	1.92	0.47
1:C:33:ASP:O	1:C:75:SER:OG	2.27	0.47
1:C:80:GLU:CG	1:C:110:LYS:HD2	2.45	0.47
2:E:109:ILE:HA	2:E:113:ALA:O	2.14	0.47
1:A:84:TRP:HE3	1:A:84:TRP:HA	1.78	0.47
1:B:224:VAL:O	1:B:224:VAL:CG1	2.61	0.47
2:E:332:ALA:HB3	2:E:333:LYS:HZ3	1.79	0.47
1:A:84:TRP:HA	1:A:84:TRP:CE3	2.49	0.47
1:B:162:LYS:HD3	1:B:270:MET:HE1	1.95	0.47
1:C:177:THR:O	1:C:177:THR:HG23	2.14	0.47
6:C:405:NAD:H2N	6:C:405:NAD:H2D	1.82	0.47
1:D:163:VAL:HG21	1:D:262:MET:CE	2.44	0.47
1:D:173:GLY:HA2	1:D:246:THR:O	2.15	0.47
2:E:203:MET:HG2	1:H:203:MET:HG2	1.96	0.47
1:G:244:ASP:OD2	1:G:309:LYS:HE3	2.14	0.47
1:H:80:GLU:OE2	1:H:107:LYS:HA	2.15	0.47
1:H:162:LYS:HD3	1:H:270:MET:HE3	1.95	0.47
1:B:103:VAL:HG11	1:G:62:LYS:HD2	1.97	0.47
1:D:109:ILE:HD12	1:D:146:ILE:HD11	1.97	0.47
1:G:194:LYS:HG3	1:G:195:ASP:H	1.79	0.47
1:A:36:THR:CG2	1:A:37:PRO:CD	2.93	0.47
1:D:273:ILE:CD1	3:D:402:PEG:H22	2.45	0.47
1:F:196:PHE:HB3	1:G:42:TYR:CE2	2.49	0.47
1:G:115:LYS:CE	1:G:145:HIS:HA	2.44	0.47
1:H:13:GLY:O	1:H:16:VAL:HG22	2.14	0.47
1:H:172:GLU:HG2	1:H:248:ARG:HB3	1.97	0.47
1:H:215:LYS:O	1:H:219:LEU:HD13	2.14	0.47
1:D:163:VAL:CG2	1:D:262:MET:CE	2.93	0.47
2:E:106:GLU:OE2	2:E:146:ILE:HD12	2.14	0.47
1:F:76:GLU:HG2	1:F:81:LYS:HB2	1.96	0.47
1:G:175:MET:O	1:G:230:GLY:HA2	2.15	0.47
1:C:171:GLU:O	1:C:227:LYS:HD2	2.15	0.46
1:B:83:PRO:HD3	7:B:504:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ILE:HG12	1:C:309:LYS:HB3	1.98	0.46
1:C:333:LYS:O	1:C:334:LYS:HB2	2.14	0.46
1:F:301:ILE:HG12	1:F:309:LYS:HB3	1.98	0.46
1:C:37:PRO:HG3	1:C:73:CYS:CB	2.45	0.46
2:E:175:MET:HG3	2:E:230:GLY:CA	2.44	0.46
1:H:137:GLU:HA	1:H:330:TYR:OH	2.16	0.46
1:H:165:LEU:HD21	1:H:223:GLU:HB2	1.97	0.46
1:A:79:PRO:HA	1:A:82:LEU:CD1	2.45	0.46
1:C:216:ALA:O	1:C:219:LEU:HB2	2.16	0.46
1:D:80:GLU:HG3	1:D:107:LYS:HG2	1.98	0.46
2:E:36:THR:OG1	2:E:38:ASP:OD1	2.33	0.46
1:A:211:THR:HA	4:A:407:GOL:H12	1.98	0.46
1:C:158:ALA:HB3	1:C:159:PRO:HD3	1.98	0.46
2:E:231:MET:HE3	2:E:231:MET:HB2	1.37	0.46
1:B:16:VAL:HG11	1:B:93:ILE:HD13	1.96	0.46
1:F:293:SER:OG	1:F:312:SER:OG	2.30	0.46
1:C:65:ILE:HA	1:C:69:LYS:O	2.16	0.46
2:E:109:ILE:HD11	2:E:146:ILE:CG1	2.46	0.46
1:D:167:ASN:HB2	1:D:168:TRP:CZ3	2.51	0.46
1:F:39:ASN:HD21	1:G:192:SER:N	1.95	0.46
1:A:60:THR:CG2	1:A:61:GLU:H	2.29	0.46
1:C:159:PRO:HA	1:C:270:MET:CE	2.46	0.46
1:G:128:PRO:HB2	1:G:130:PHE:CE2	2.51	0.46
1:G:217:VAL:CG1	1:G:228:LEU:HD11	2.46	0.46
1:D:84:TRP:HA	1:D:84:TRP:HE3	1.80	0.45
1:H:36:THR:OG1	1:H:38:ASP:OD1	2.30	0.45
2:E:197:ARG:NH2	1:F:298:ASP:HB3	2.30	0.45
1:F:252:GLU:CB	1:F:305:SER:OG	2.63	0.45
1:F:266:SER:O	1:F:271:LYS:HA	2.16	0.45
1:H:17:PHE:CZ	1:H:21:ILE:HD13	2.51	0.45
1:A:248:ARG:HA	1:A:306:ARG:O	2.15	0.45
1:G:3:ARG:NH1	1:G:27:GLU:OE2	2.50	0.45
1:D:218:GLY:HA2	1:D:224:VAL:HG23	1.98	0.45
1:G:253:THR:OG1	1:G:257:GLU:OE1	2.28	0.45
1:A:224:VAL:HA	1:A:227:LYS:HE3	1.99	0.45
1:D:17:PHE:HZ	1:D:71:ILE:HD13	1.80	0.45
1:F:253:THR:OG1	1:F:257:GLU:OE1	2.31	0.45
1:H:255:LEU:HD21	1:H:300:CYS:HB3	1.98	0.45
1:B:65:ILE:HA	1:B:69:LYS:O	2.15	0.45
1:B:165:LEU:HD12	1:B:169:GLY:HA2	1.97	0.45
1:C:123:LYS:HE2	1:C:123:LYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:301:ILE:HG12	2:E:309:LYS:HB3	1.99	0.45
1:C:171:GLU:O	1:C:172:GLU:HG3	2.17	0.45
1:C:179:HIS:HB3	1:C:234:ARG:HD3	1.98	0.45
1:D:101:ASP:OD1	1:D:104:GLY:N	2.42	0.45
1:F:252:GLU:HB3	1:F:305:SER:HG	1.82	0.45
1:H:222:PRO:HD2	7:H:504:HOH:O	2.17	0.45
1:C:284:ASN:HB2	1:D:205:ASN:OD1	2.17	0.45
1:D:152:CSD:OD2	1:D:316:ASN:HB2	2.17	0.45
1:G:115:LYS:HE2	1:G:145:HIS:HA	1.99	0.45
1:G:248:ARG:HD2	1:G:307:PHE:HZ	1.79	0.45
1:B:178:ILE:N	1:B:178:ILE:HD12	2.31	0.44
1:C:33:ASP:O	1:C:75:SER:HA	2.17	0.44
1:C:168:TRP:CZ2	1:C:257:GLU:HG2	2.52	0.44
1:C:214:ALA:O	1:C:228:LEU:CD1	2.63	0.44
2:E:30:ALA:HA	2:E:72:LEU:O	2.17	0.44
1:F:23:ASP:OD2	1:F:329:ARG:NH1	2.49	0.44
1:H:248:ARG:CD	1:H:307:PHE:CZ	3.00	0.44
1:B:117:VAL:CG2	1:B:331:MET:HE1	2.47	0.44
1:B:117:VAL:HG21	1:B:331:MET:HE1	1.98	0.44
1:B:326:ASP:OD1	1:B:329:ARG:NH1	2.50	0.44
2:E:33:ASP:O	2:E:75:SER:HA	2.17	0.44
1:G:33:ASP:O	1:G:75:SER:HA	2.17	0.44
1:G:78:ASP:OD2	1:G:80:GLU:CD	2.60	0.44
1:A:196:PHE:HB3	1:D:42:TYR:CE2	2.53	0.44
1:B:224:VAL:CG1	1:B:228:LEU:HG	2.47	0.44
2:E:11:ARG:O	2:E:15:LEU:HG	2.17	0.44
2:E:205:ASN:OD1	1:F:284:ASN:HB2	2.17	0.44
1:F:64:LEU:HD13	1:F:73:CYS:SG	2.57	0.44
4:H:403:GOL:H32	6:H:406:NAD:C3N	2.48	0.44
1:A:212:GLY:N	4:A:407:GOL:O1	2.49	0.44
1:A:323:ARG:HA	1:A:323:ARG:NE	2.32	0.44
1:A:224:VAL:HG22	1:A:228:LEU:HG	2.00	0.44
1:C:214:ALA:O	1:C:217:VAL:HG12	2.17	0.44
2:E:80:GLU:HG3	2:E:107:LYS:HB3	2.00	0.44
1:H:171:GLU:C	1:H:172:GLU:OE1	2.60	0.44
1:H:234:ARG:NH2	4:H:403:GOL:H11	2.33	0.44
1:H:240:VAL:HG11	1:H:283:SER:O	2.18	0.44
1:G:244:ASP:OD1	1:G:309:LYS:HG2	2.17	0.44
1:A:284:ASN:HB2	1:B:205:ASN:OD1	2.18	0.44
1:B:290:THR:CG2	3:B:402:PEG:H22	2.45	0.44
1:C:323:ARG:HA	1:C:323:ARG:HD3	1.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:THR:OG1	4:D:404:GOL:H12	2.16	0.44
1:F:164:VAL:HG12	1:F:170:ILE:CG1	2.48	0.44
1:G:243:VAL:HG23	1:G:314:TYR:HE1	1.83	0.44
1:H:245:LEU:HG	1:H:247:VAL:HG22	1.98	0.44
1:H:259:SER:OG	1:H:297:MET:HG3	2.18	0.44
1:A:173:GLY:HA3	1:A:228:LEU:CD2	2.48	0.44
1:C:231:MET:HE3	1:C:231:MET:HB2	1.58	0.44
1:F:162:LYS:HD3	1:F:270:MET:HE1	1.99	0.44
1:H:85:LYS:HE2	1:H:85:LYS:HB2	1.46	0.44
1:H:261:LYS:HA	1:H:261:LYS:HD3	1.73	0.44
1:C:168:TRP:CH2	1:C:258:ILE:HA	2.53	0.43
2:E:248:ARG:HD2	2:E:307:PHE:CE1	2.52	0.43
1:F:252:GLU:CG	1:F:306:ARG:NH1	2.81	0.43
1:A:35:VAL:HG23	1:A:40:LEU:CD2	2.48	0.43
1:A:58:GLU:HB2	1:A:65:ILE:HB	2.00	0.43
1:C:286:PHE:CD1	1:C:294:ILE:HD13	2.53	0.43
1:D:241:SER:HB2	1:D:314:TYR:CZ	2.52	0.43
2:E:94:GLU:HB3	2:E:118:ILE:HA	2.00	0.43
1:G:10:GLY:O	1:G:14:ARG:HG3	2.19	0.43
1:H:241:SER:HB2	1:H:314:TYR:CZ	2.53	0.43
1:B:35:VAL:HG11	1:C:191:PRO:HB3	2.00	0.43
1:B:168:TRP:CA	1:B:251:LYS:HE3	2.39	0.43
1:F:287:VAL:O	1:F:288:SER:HB2	2.18	0.43
1:F:297:MET:HE3	1:F:297:MET:HB3	1.88	0.43
1:A:158:ALA:HB2	1:A:217:VAL:HG22	2.00	0.43
1:D:244:ASP:OD1	1:D:309:LYS:CG	2.66	0.43
1:G:309:LYS:CD	1:H:231:MET:CE	2.88	0.43
1:H:275:GLY:HA3	1:H:291:LEU:HD13	2.00	0.43
1:A:36:THR:HG22	1:A:37:PRO:CD	2.45	0.43
1:A:205:ASN:OD1	1:B:284:ASN:HB2	2.18	0.43
2:E:174:LEU:HD12	2:E:174:LEU:N	2.34	0.43
1:F:137:GLU:HA	1:F:330:TYR:OH	2.18	0.43
1:A:278:GLU:CG	1:A:297:MET:CE	2.96	0.43
1:B:10:GLY:HA3	6:B:412:NAD:H52A	2.00	0.43
1:B:248:ARG:HA	1:B:306:ARG:O	2.18	0.43
1:D:218:GLY:O	1:D:222:PRO:HA	2.18	0.43
2:E:250:THR:HA	2:E:306:ARG:HH21	1.83	0.43
1:F:168:TRP:CH2	1:F:258:ILE:HA	2.54	0.43
1:B:9:PHE:CE2	1:B:14:ARG:HG2	2.53	0.43
1:F:23:ASP:HA	1:F:24:PRO:HD3	1.89	0.43
1:H:94:GLU:HB3	1:H:118:ILE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:GLU:H	1:C:137:GLU:CD	2.25	0.43
2:E:98:LEU:HD12	6:E:403:NAD:N7A	2.33	0.43
1:F:3:ARG:HD3	1:F:88:LYS:O	2.18	0.43
1:B:301:ILE:HG12	1:B:309:LYS:HB3	2.00	0.43
1:D:223:GLU:H	1:D:223:GLU:CD	2.15	0.43
2:E:329:ARG:HA	2:E:333:LYS:HZ3	1.84	0.43
1:G:173:GLY:O	1:G:228:LEU:HA	2.19	0.43
1:A:11:ARG:HH11	1:A:14:ARG:HH21	1.67	0.42
1:A:281:VAL:O	1:B:197:ARG:NH1	2.50	0.42
1:B:244[A]:ASP:OD2	1:B:309:LYS:HE3	2.18	0.42
2:E:12:ILE:O	2:E:16:VAL:HG22	2.18	0.42
2:E:329:ARG:O	2:E:333:LYS:NZ	2.51	0.42
1:H:80:GLU:OE2	1:H:107:LYS:CG	2.56	0.42
1:H:175:MET:O	1:H:230:GLY:HA2	2.19	0.42
1:H:239:ASP:O	1:H:240:VAL:HB	2.19	0.42
1:A:11:ARG:HH11	1:A:14:ARG:NH2	2.18	0.42
1:D:172:GLU:OE2	1:D:248:ARG:HD3	2.19	0.42
1:C:63:GLU:HB2	1:C:71:ILE:O	2.19	0.42
1:D:179:HIS:CD2	4:D:404:GOL:H31	2.54	0.42
1:G:56:THR:HG22	1:G:67:ASP:HA	2.01	0.42
1:G:174:LEU:HG	1:G:229:THR:HG22	2.01	0.42
2:E:34:LEU:HD21	2:E:77:ARG:CG	2.42	0.42
2:E:291:LEU:HD12	2:E:294:ILE:HG12	2.02	0.42
1:B:1:MET:HE3	1:B:1:MET:HB2	1.85	0.42
1:B:103:VAL:HG21	1:G:62:LYS:HB3	2.01	0.42
1:B:333:LYS:O	1:B:334:LYS:HB3	2.20	0.42
1:G:174:LEU:HD22	1:H:246:THR:HG23	2.01	0.42
1:G:217:VAL:CG1	1:G:228:LEU:HD21	2.47	0.42
1:H:3:ARG:NH1	1:H:87:LEU:O	2.52	0.42
1:A:215:LYS:O	1:A:218:GLY:N	2.52	0.42
2:E:173:GLY:HA2	2:E:246:THR:O	2.19	0.42
1:A:10:GLY:HA3	6:A:411:NAD:O5B	2.19	0.42
1:D:84:TRP:CE3	1:D:84:TRP:CA	3.03	0.42
1:H:128:PRO:HG2	1:H:147:VAL:HG12	2.02	0.42
1:F:11:ARG:O	1:F:15:LEU:HG	2.20	0.42
1:F:106:GLU:CD	1:F:110:LYS:HG3	2.44	0.42
1:H:175:MET:CE	1:H:243:VAL:HG22	2.48	0.42
1:A:286:PHE:HE1	1:A:294:ILE:HG21	1.83	0.42
1:C:248:ARG:HD2	1:C:307:PHE:HZ	1.78	0.42
1:D:65:ILE:HG12	1:D:70:LYS:HG2	2.01	0.42
1:D:175:MET:HE2	1:D:175:MET:HB2	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:LYS:CD	1:F:145:HIS:HA	2.50	0.42
1:C:197:ARG:HG3	1:D:280:MET:HB3	2.02	0.42
1:D:234:ARG:HH22	4:D:405:GOL:C3	2.33	0.42
2:E:179:HIS:HB3	2:E:234:ARG:HD3	2.02	0.42
1:F:84:TRP:CE3	1:F:84:TRP:CA	3.03	0.42
1:G:1:MET:HB2	1:G:1:MET:HE3	1.70	0.42
1:G:15:LEU:CD1	1:G:317:GLU:HB3	2.50	0.42
1:C:280:MET:HB3	1:D:197:ARG:HG3	2.02	0.41
1:D:123:LYS:HE3	7:D:503:HOH:O	2.20	0.41
2:E:102:ARG:O	2:E:106:GLU:CG	2.68	0.41
2:E:280:MET:HE1	2:E:298:ASP:OD2	2.20	0.41
1:F:329:ARG:NH2	7:F:502:HOH:O	2.52	0.41
1:G:17:PHE:CZ	1:G:71:ILE:HD13	2.54	0.41
1:A:65:ILE:O	1:A:65:ILE:HG22	2.18	0.41
1:A:278:GLU:HG2	1:A:297:MET:HE2	2.01	0.41
2:E:128:PRO:HG2	2:E:147:VAL:HG12	2.02	0.41
1:H:248:ARG:CD	1:H:307:PHE:CE1	3.03	0.41
1:A:255:LEU:HD21	1:A:300:CYS:HB3	2.02	0.41
1:B:131:VAL:HG13	1:B:155:ASN:OD1	2.21	0.41
1:C:56:THR:HG23	1:C:56:THR:O	2.21	0.41
2:E:11:ARG:HH11	2:E:14:ARG:HH21	1.68	0.41
1:A:257:GLU:OE2	2:E:257:GLU:OE1	2.37	0.41
1:D:175:MET:CE	1:D:243:VAL:HG13	2.50	0.41
1:F:192:SER:H	1:G:39:ASN:ND2	2.11	0.41
1:B:16:VAL:HG11	1:B:93:ILE:CD1	2.50	0.41
1:B:124[A]:ASP:N	1:B:124[A]:ASP:OD1	2.53	0.41
1:B:256:LYS:HB3	1:B:256:LYS:HE2	1.42	0.41
2:E:224:VAL:HA	2:E:227:LYS:HD2	2.02	0.41
1:B:11:ARG:O	1:B:15:LEU:HG	2.19	0.41
1:B:272:GLY:O	1:B:323:ARG:NH2	2.54	0.41
1:C:234:ARG:HH21	4:C:402:GOL:H12	1.85	0.41
1:A:13:GLY:O	1:A:16:VAL:HG22	2.21	0.41
1:A:41:ALA:HB2	1:A:64:LEU:CD2	2.51	0.41
1:B:74:VAL:HG21	1:B:82:LEU:HD22	2.02	0.41
1:C:115:LYS:NZ	1:C:144:ASP:O	2.50	0.41
1:C:235:VAL:HA	1:C:236:PRO:HD3	1.88	0.41
2:E:132:MET:HE2	2:E:326:ASP:HB3	2.01	0.41
1:F:292:SER:OG	1:F:323:ARG:HD2	2.21	0.41
1:G:17:PHE:CE1	1:G:71:ILE:HD13	2.55	0.41
1:A:261:LYS:HD3	1:A:261:LYS:HA	1.89	0.41
1:B:173:GLY:HA2	1:B:246:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:405:GOL:H11	6:D:410:NAD:N1N	2.36	0.41
2:E:139:TYR:CZ	2:E:141:PRO:HA	2.56	0.41
2:E:331:MET:HE3	2:E:331:MET:HB2	1.83	0.41
1:B:173:GLY:O	1:B:228:LEU:HA	2.21	0.41
1:C:128:PRO:HG3	1:C:144:ASP:CG	2.46	0.41
1:F:91:TYR:HE1	1:F:331:MET:CE	2.29	0.41
1:G:108:HIS:HB2	1:G:116:VAL:HG21	2.03	0.41
1:A:15:LEU:CD1	1:A:317:GLU:HB3	2.51	0.41
1:B:94:GLU:HG2	1:B:108:HIS:HE2	1.86	0.41
1:B:175:MET:HG3	1:B:230:GLY:HA3	2.01	0.41
1:F:323:ARG:NE	1:F:323:ARG:HA	2.36	0.41
1:G:171:GLU:C	1:G:172:GLU:CD	2.88	0.41
1:A:278:GLU:CG	1:A:297:MET:HE3	2.52	0.40
2:E:15:LEU:HD12	2:E:317:GLU:HB3	2.01	0.40
2:E:77:ARG:O	2:E:79:PRO:HD3	2.21	0.40
2:E:246:THR:HG23	1:F:174:LEU:HD22	2.03	0.40
1:F:219:LEU:HD23	1:F:219:LEU:HA	1.88	0.40
1:G:78:ASP:OD2	1:G:80:GLU:HG3	2.21	0.40
1:H:115:LYS:CD	1:H:145:HIS:HA	2.51	0.40
1:A:284:ASN:HA	1:A:287:VAL:HG23	2.04	0.40
1:A:45:LYS:O	1:A:52:ARG:HA	2.21	0.40
1:A:241:SER:HB2	1:A:314:TYR:CZ	2.55	0.40
1:D:165:LEU:HD23	1:D:166:ASP:OD1	2.20	0.40
1:F:3:ARG:NH1	1:F:27:GLU:OE1	2.54	0.40
1:G:248:ARG:HA	1:G:306:ARG:O	2.22	0.40
1:H:56:THR:CG2	1:H:67:ASP:HA	2.52	0.40
1:H:301:ILE:HD13	1:H:301:ILE:HG21	1.89	0.40
1:A:256:LYS:NZ	3:A:402:PEG:O2	2.50	0.40
1:B:290:THR:H	3:B:402:PEG:C2	2.29	0.40
1:G:10:GLY:HA3	6:G:401:NAD:O5B	2.22	0.40
1:H:316:ASN:ND2	1:H:316:ASN:H	2.20	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	331/337 (98%)	323 (98%)	6 (2%)	2 (1%)	21	30
1	B	335/337 (99%)	329 (98%)	5 (2%)	1 (0%)	36	48
1	C	331/337 (98%)	325 (98%)	5 (2%)	1 (0%)	36	48
1	D	330/337 (98%)	324 (98%)	5 (2%)	1 (0%)	36	48
1	F	332/337 (98%)	324 (98%)	7 (2%)	1 (0%)	36	48
1	G	331/337 (98%)	321 (97%)	9 (3%)	1 (0%)	36	48
1	H	331/337 (98%)	327 (99%)	3 (1%)	1 (0%)	36	48
2	E	332/337 (98%)	323 (97%)	8 (2%)	1 (0%)	36	48
All	All	2653/2696 (98%)	2596 (98%)	48 (2%)	9 (0%)	36	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	240	VAL
2	E	240	VAL
1	F	240	VAL
1	H	240	VAL
1	A	240	VAL
1	B	240	VAL
1	D	240	VAL
1	G	240	VAL
1	A	333	LYS

5.3.2 Protein sidechains [i](#)

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	284/284 (100%)	282 (99%)	2 (1%)	76	87
1	B	286/284 (101%)	283 (99%)	3 (1%)	68	82
1	C	284/284 (100%)	282 (99%)	2 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	283/284 (100%)	279 (99%)	4 (1%)	59	77
1	F	284/284 (100%)	281 (99%)	3 (1%)	65	81
1	G	284/284 (100%)	281 (99%)	3 (1%)	65	81
1	H	283/284 (100%)	279 (99%)	4 (1%)	59	77
2	E	285/285 (100%)	282 (99%)	3 (1%)	65	81
All	All	2273/2273 (100%)	2249 (99%)	24 (1%)	65	81

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	TRP
1	A	224	VAL
1	B	84	TRP
1	B	247	VAL
1	B	307	PHE
1	C	60	THR
1	C	323	ARG
1	D	36	THR
1	D	84	TRP
1	D	184	THR
1	D	228	LEU
2	E	73	CYS
2	E	217	VAL
2	E	246	THR
1	F	84	TRP
1	F	184	THR
1	F	247	VAL
1	G	176	THR
1	G	203	MET
1	G	228	LEU
1	H	40	LEU
1	H	172	GLU
1	H	224	VAL
1	H	316	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN

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Mol	Chain	Res	Type
1	A	39	ASN
1	A	155	ASN
1	A	167	ASN
1	A	225	ASN
1	A	322	ASN
1	B	39	ASN
1	B	204	GLN
1	C	39	ASN
1	C	145	HIS
1	D	39	ASN
1	D	204	GLN
2	E	39	ASN
2	E	322	ASN
1	F	39	ASN
1	F	225	ASN
1	G	39	ASN
1	G	179	HIS
1	G	204	GLN
1	H	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSD	C	152	1	4,7,8	1.03	0	1,8,10	0.14	0
1	CSD	B	152	1	4,7,8	1.09	0	1,8,10	0.85	0
1	CSD	F	152	1	4,7,8	1.00	0	1,8,10	0.81	0
1	CSD	A	152	1	4,7,8	0.99	0	1,8,10	1.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	G	152	1	4,7,8	0.83	0	1,8,10	0.11	0
1	CSD	D	152	1	4,7,8	0.99	0	1,8,10	0.41	0
1	CSD	H	152	1	4,7,8	0.91	0	1,8,10	0.23	0

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
1	CSD	C	152	1	-	0/2/6/8	-
1	CSD	B	152	1	-	1/2/6/8	-
1	CSD	F	152	1	-	0/2/6/8	-
1	CSD	A	152	1	-	0/2/6/8	-
1	CSD	G	152	1	-	0/2/6/8	-
1	CSD	D	152	1	-	0/2/6/8	-
1	CSD	H	152	1	-	0/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	152	CSD	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	152	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

52 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	B	405	-	5,5,5	0.30	0	5,5,5	0.99	0
3	PEG	D	402	-	6,6,6	0.32	0	5,5,5	0.29	0
4	GOL	D	403	-	5,5,5	0.26	0	5,5,5	0.96	0
4	GOL	B	409	-	5,5,5	0.53	0	5,5,5	0.43	0
4	GOL	H	405	-	5,5,5	0.27	0	5,5,5	0.44	0
6	NAD	H	406	-	46,48,48	0.82	2 (4%)	64,73,73	0.70	1 (1%)
4	GOL	H	404	-	5,5,5	0.24	0	5,5,5	0.82	0
5	PO4	A	410	-	4,4,4	1.80	1 (25%)	6,6,6	0.66	0
4	GOL	A	407	-	5,5,5	0.27	0	5,5,5	0.84	0
4	GOL	B	408	-	5,5,5	0.22	0	5,5,5	0.65	0
4	GOL	A	406	-	5,5,5	0.42	0	5,5,5	0.69	0
4	GOL	H	402	-	5,5,5	0.27	0	5,5,5	0.72	0
4	GOL	B	404	-	5,5,5	0.28	0	5,5,5	0.59	0
6	NAD	B	412	-	46,48,48	0.84	1 (2%)	64,73,73	1.15	5 (7%)
6	NAD	D	410	-	46,48,48	0.67	1 (2%)	64,73,73	1.43	6 (9%)
5	PO4	B	410	-	4,4,4	1.89	1 (25%)	6,6,6	0.79	0
4	GOL	D	407	-	5,5,5	0.31	0	5,5,5	0.56	0
4	GOL	A	413	-	5,5,5	0.25	0	5,5,5	0.36	0
4	GOL	D	405	-	5,5,5	0.35	0	5,5,5	0.94	0
4	GOL	A	408	-	5,5,5	0.29	0	5,5,5	0.51	0
4	GOL	D	408	-	5,5,5	0.18	0	5,5,5	0.77	0
6	NAD	G	401	-	46,48,48	0.93	2 (4%)	64,73,73	1.44	6 (9%)
4	GOL	B	406	-	5,5,5	0.29	0	5,5,5	0.38	0
4	GOL	D	404	-	5,5,5	0.23	0	5,5,5	0.58	0
6	NAD	C	405	-	46,48,48	0.90	1 (2%)	64,73,73	0.97	4 (6%)
4	GOL	C	404	-	5,5,5	0.22	0	5,5,5	0.70	0
3	PEG	B	403	-	6,6,6	0.31	0	5,5,5	0.29	0
3	PEG	H	401	-	6,6,6	0.26	0	5,5,5	0.29	0
3	PEG	B	401	-	6,6,6	0.39	0	5,5,5	0.51	0
4	GOL	C	401	-	5,5,5	0.33	0	5,5,5	0.41	0
3	PEG	A	401	-	6,6,6	0.33	0	5,5,5	0.30	0
4	GOL	A	405	-	5,5,5	0.31	0	5,5,5	0.52	0
4	GOL	C	403	-	5,5,5	0.24	0	5,5,5	0.76	0
4	GOL	D	406	-	5,5,5	0.32	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	F	401	-	5,5,5	0.32	0	5,5,5	0.61	0
4	GOL	A	403	-	5,5,5	0.27	0	5,5,5	1.08	0
4	GOL	E	401	-	5,5,5	0.25	0	5,5,5	0.34	0
4	GOL	E	402	-	5,5,5	0.28	0	5,5,5	0.49	0
4	GOL	D	401	-	5,5,5	0.20	0	5,5,5	0.40	0
6	NAD	E	403	-	46,48,48	0.60	1 (2%)	64,73,73	0.68	1 (1%)
4	GOL	C	402	-	5,5,5	0.41	0	5,5,5	0.48	0
4	GOL	A	412	-	5,5,5	0.26	0	5,5,5	0.59	0
3	PEG	A	402	-	6,6,6	0.34	0	5,5,5	0.40	0
4	GOL	A	404	-	5,5,5	0.33	0	5,5,5	0.61	0
5	PO4	B	411	-	4,4,4	1.86	1 (25%)	6,6,6	0.57	0
4	GOL	H	403	-	5,5,5	0.28	0	5,5,5	0.51	0
6	NAD	A	411	-	46,48,48	0.76	1 (2%)	64,73,73	1.11	7 (10%)
6	NAD	F	402	-	46,48,48	0.61	1 (2%)	64,73,73	0.88	3 (4%)
5	PO4	D	409	-	4,4,4	1.77	1 (25%)	6,6,6	0.79	0
3	PEG	B	402	-	6,6,6	0.34	0	5,5,5	0.63	0
4	GOL	A	409	-	5,5,5	0.30	0	5,5,5	0.45	0
4	GOL	B	407	-	5,5,5	0.33	0	5,5,5	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	405	-	-	4/4/4/4	-
3	PEG	D	402	-	-	2/4/4/4	-
4	GOL	D	403	-	-	3/4/4/4	-
4	GOL	B	409	-	-	4/4/4/4	-
4	GOL	H	405	-	-	1/4/4/4	-
6	NAD	H	406	-	-	6/30/62/62	0/5/5/5
4	GOL	H	404	-	-	0/4/4/4	-
4	GOL	A	407	-	-	2/4/4/4	-
4	GOL	B	408	-	-	4/4/4/4	-
4	GOL	A	406	-	-	2/4/4/4	-
4	GOL	H	402	-	-	0/4/4/4	-
4	GOL	B	404	-	-	4/4/4/4	-
6	NAD	B	412	-	-	6/30/62/62	0/5/5/5
6	NAD	D	410	-	-	4/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	407	-	-	2/4/4/4	-
4	GOL	A	413	-	-	0/4/4/4	-
4	GOL	D	405	-	-	3/4/4/4	-
4	GOL	A	408	-	-	0/4/4/4	-
4	GOL	D	408	-	-	0/4/4/4	-
6	NAD	G	401	-	-	5/30/62/62	0/5/5/5
4	GOL	B	406	-	-	0/4/4/4	-
4	GOL	D	404	-	-	0/4/4/4	-
6	NAD	C	405	-	-	4/30/62/62	0/5/5/5
4	GOL	C	404	-	-	4/4/4/4	-
3	PEG	B	403	-	-	1/4/4/4	-
3	PEG	H	401	-	-	1/4/4/4	-
3	PEG	B	401	-	-	4/4/4/4	-
4	GOL	C	401	-	-	2/4/4/4	-
3	PEG	A	401	-	-	2/4/4/4	-
4	GOL	A	405	-	-	0/4/4/4	-
4	GOL	C	403	-	-	2/4/4/4	-
4	GOL	D	406	-	-	0/4/4/4	-
4	GOL	F	401	-	-	1/4/4/4	-
4	GOL	A	403	-	-	4/4/4/4	-
4	GOL	E	401	-	-	2/4/4/4	-
4	GOL	E	402	-	-	4/4/4/4	-
4	GOL	D	401	-	-	0/4/4/4	-
6	NAD	E	403	-	-	3/30/62/62	0/5/5/5
4	GOL	C	402	-	-	4/4/4/4	-
4	GOL	A	412	-	-	0/4/4/4	-
3	PEG	A	402	-	-	3/4/4/4	-
4	GOL	A	404	-	-	0/4/4/4	-
6	NAD	A	411	-	-	5/30/62/62	0/5/5/5
4	GOL	H	403	-	-	0/4/4/4	-
6	NAD	F	402	-	-	7/30/62/62	0/5/5/5
3	PEG	B	402	-	-	3/4/4/4	-
4	GOL	A	409	-	-	0/4/4/4	-
4	GOL	B	407	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	405	NAD	C2N-N1N	5.00	1.40	1.35
6	B	412	NAD	C2N-N1N	4.15	1.39	1.35
6	H	406	NAD	C2N-N1N	4.13	1.39	1.35
6	A	411	NAD	C2N-N1N	3.87	1.39	1.35
6	G	401	NAD	O4D-C1D	3.70	1.45	1.40
5	B	410	PO4	P-O1	3.44	1.58	1.50
6	G	401	NAD	C2N-N1N	3.21	1.38	1.35
5	A	410	PO4	P-O1	3.08	1.57	1.50
5	B	411	PO4	P-O1	3.07	1.57	1.50
5	D	409	PO4	P-O1	3.02	1.57	1.50
6	E	403	NAD	C2N-N1N	2.52	1.37	1.35
6	F	402	NAD	C2N-N1N	2.42	1.37	1.35
6	H	406	NAD	O4D-C1D	2.29	1.43	1.40
6	D	410	NAD	C2N-N1N	2.02	1.37	1.35

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	401	NAD	O2B-C2B-C1B	7.39	135.56	110.10
6	D	410	NAD	O2B-C2B-C1B	6.97	134.11	110.10
6	A	411	NAD	O2B-C2B-C1B	4.15	124.40	110.10
6	G	401	NAD	C2B-C1B-N9A	-4.03	103.30	113.30
6	D	410	NAD	C2B-C1B-N9A	-3.77	103.94	113.30
6	D	410	NAD	O3B-C3B-C4B	-3.59	100.77	111.08
6	B	412	NAD	C6N-N1N-C2N	-3.54	118.87	121.88
6	G	401	NAD	C6N-N1N-C2N	-3.29	119.08	121.88
6	D	410	NAD	C2B-C3B-C4B	3.16	108.71	102.61
6	F	402	NAD	C6N-N1N-C2N	-3.16	119.19	121.88
6	H	406	NAD	C6N-N1N-C2N	-3.15	119.20	121.88
6	C	405	NAD	O3D-C3D-C4D	-3.08	102.24	111.08
6	B	412	NAD	O2B-C2B-C1B	3.08	120.70	110.10
6	A	411	NAD	C6N-N1N-C2N	-2.98	119.34	121.88
6	B	412	NAD	O3D-C3D-C4D	-2.97	102.55	111.08
6	A	411	NAD	O3B-C3B-C4B	-2.95	102.60	111.08
6	E	403	NAD	C6N-N1N-C2N	-2.95	119.37	121.88
6	G	401	NAD	O3B-C3B-C4B	-2.94	102.64	111.08
6	C	405	NAD	C6N-N1N-C2N	-2.83	119.47	121.88
6	F	402	NAD	O2B-C2B-C1B	2.81	119.77	110.10
6	G	401	NAD	C2N-N1N-C1D	2.45	124.53	119.13
6	F	402	NAD	O3D-C3D-C4D	-2.39	104.22	111.08
6	B	412	NAD	C2B-C3B-C4B	2.34	107.12	102.61
6	C	405	NAD	C2N-N1N-C1D	2.29	124.19	119.13
6	C	405	NAD	O2D-C2D-C3D	-2.25	104.60	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	411	NAD	C2B-C1B-N9A	-2.20	107.83	113.30
6	D	410	NAD	O3D-C3D-C4D	-2.17	104.83	111.08
6	G	401	NAD	O3D-C3D-C4D	-2.14	104.93	111.08
6	D	410	NAD	C6N-N1N-C2N	-2.09	120.10	121.88
6	A	411	NAD	O2A-PA-O1A	2.07	122.09	112.44
6	A	411	NAD	C2B-C3B-C4B	2.05	106.57	102.61
6	A	411	NAD	C4D-O4D-C1D	-2.01	108.08	109.92
6	B	412	NAD	O2A-PA-O1A	2.01	121.78	112.44

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	GOL	O1-C1-C2-C3
4	A	406	GOL	C1-C2-C3-O3
4	A	407	GOL	O1-C1-C2-O2
4	A	407	GOL	O1-C1-C2-C3
4	B	404	GOL	C1-C2-C3-O3
4	B	405	GOL	C1-C2-C3-O3
4	B	408	GOL	O1-C1-C2-C3
4	B	408	GOL	C1-C2-C3-O3
4	B	409	GOL	C1-C2-C3-O3
4	C	401	GOL	C1-C2-C3-O3
4	C	402	GOL	O1-C1-C2-C3
4	C	403	GOL	O1-C1-C2-C3
4	C	404	GOL	O1-C1-C2-O2
4	C	404	GOL	O1-C1-C2-C3
4	D	405	GOL	O1-C1-C2-C3
4	D	407	GOL	O1-C1-C2-C3
4	E	401	GOL	C1-C2-C3-O3
4	E	402	GOL	C1-C2-C3-O3
6	A	411	NAD	O4D-C1D-N1N-C2N
6	A	411	NAD	O4D-C1D-N1N-C6N
6	A	411	NAD	C2D-C1D-N1N-C2N
6	A	411	NAD	C2D-C1D-N1N-C6N
6	B	412	NAD	O4D-C1D-N1N-C2N
6	C	405	NAD	O4D-C1D-N1N-C2N
6	C	405	NAD	O4D-C1D-N1N-C6N
6	C	405	NAD	C2D-C1D-N1N-C2N
6	C	405	NAD	C2D-C1D-N1N-C6N
6	D	410	NAD	O4D-C1D-N1N-C2N
6	D	410	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
6	D	410	NAD	C2D-C1D-N1N-C2N
6	D	410	NAD	C2D-C1D-N1N-C6N
6	E	403	NAD	O4D-C1D-N1N-C2N
6	F	402	NAD	O4D-C1D-N1N-C2N
6	F	402	NAD	O4D-C1D-N1N-C6N
6	F	402	NAD	C2D-C1D-N1N-C2N
6	F	402	NAD	C2D-C1D-N1N-C6N
6	G	401	NAD	O4D-C1D-N1N-C2N
6	G	401	NAD	O4D-C1D-N1N-C6N
6	G	401	NAD	C2D-C1D-N1N-C2N
6	G	401	NAD	C2D-C1D-N1N-C6N
6	H	406	NAD	O4D-C1D-N1N-C2N
6	H	406	NAD	O4D-C1D-N1N-C6N
6	H	406	NAD	C2D-C1D-N1N-C2N
6	H	406	NAD	C2D-C1D-N1N-C6N
4	B	409	GOL	O2-C2-C3-O3
4	C	401	GOL	O2-C2-C3-O3
4	E	402	GOL	O1-C1-C2-O2
3	A	402	PEG	O2-C3-C4-O4
3	A	401	PEG	O1-C1-C2-O2
3	B	403	PEG	O2-C3-C4-O4
4	A	403	GOL	C1-C2-C3-O3
4	B	404	GOL	O1-C1-C2-C3
4	B	407	GOL	O1-C1-C2-C3
4	B	409	GOL	O1-C1-C2-C3
4	C	402	GOL	C1-C2-C3-O3
4	C	404	GOL	C1-C2-C3-O3
4	D	403	GOL	O1-C1-C2-C3
4	D	403	GOL	C1-C2-C3-O3
4	E	402	GOL	O1-C1-C2-C3
4	F	401	GOL	O1-C1-C2-C3
4	B	404	GOL	O2-C2-C3-O3
4	B	405	GOL	O2-C2-C3-O3
4	B	407	GOL	O1-C1-C2-O2
4	C	402	GOL	O1-C1-C2-O2
4	C	403	GOL	O1-C1-C2-O2
4	D	403	GOL	O2-C2-C3-O3
4	D	405	GOL	O1-C1-C2-O2
4	D	407	GOL	O1-C1-C2-O2
4	E	401	GOL	O2-C2-C3-O3
4	E	402	GOL	O2-C2-C3-O3
3	A	401	PEG	O2-C3-C4-O4

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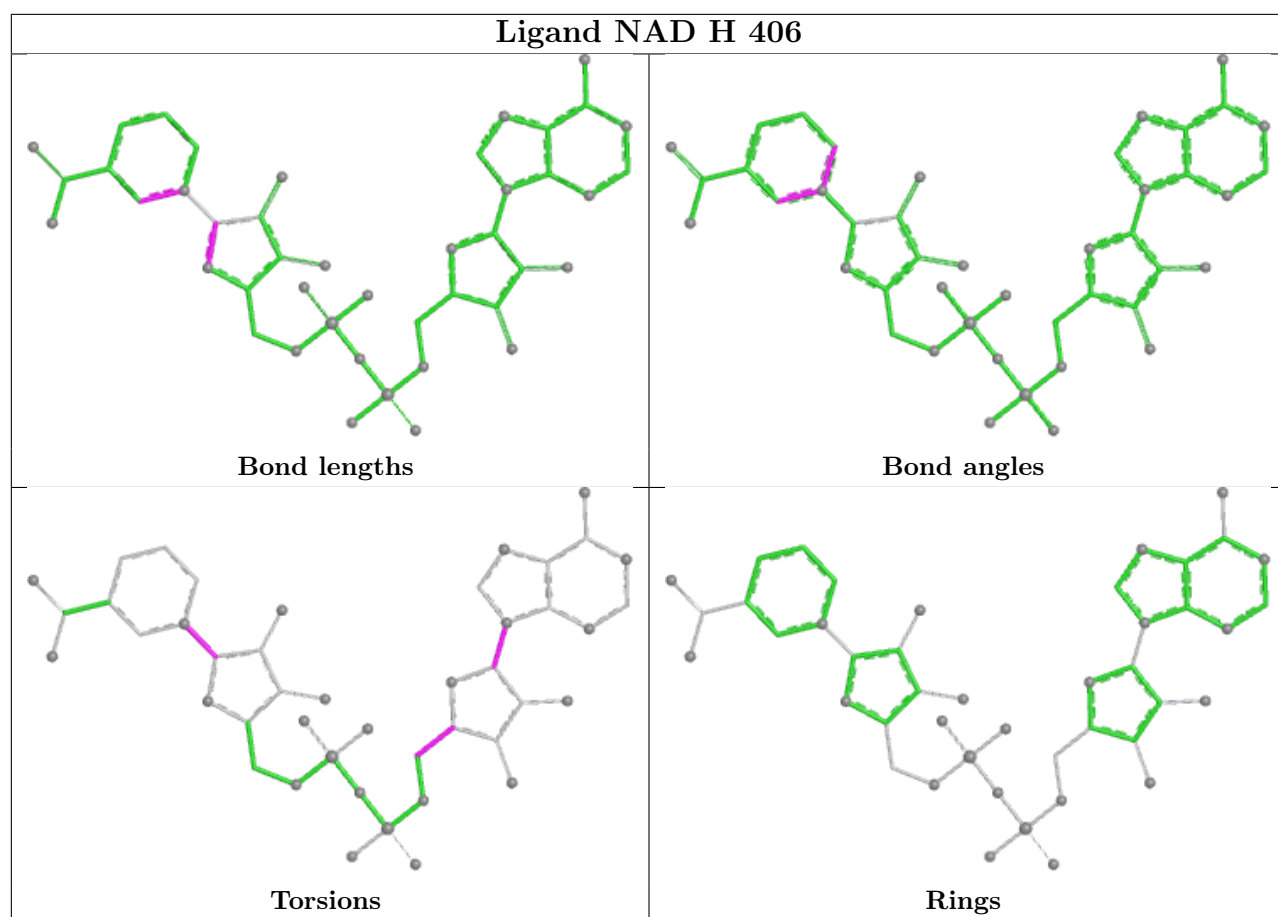
Mol	Chain	Res	Type	Atoms
6	B	412	NAD	O4B-C4B-C5B-O5B
6	B	412	NAD	C3B-C4B-C5B-O5B
3	B	401	PEG	O2-C3-C4-O4
4	A	403	GOL	O1-C1-C2-O2
4	A	406	GOL	O2-C2-C3-O3
4	B	408	GOL	O2-C2-C3-O3
4	C	404	GOL	O2-C2-C3-O3
3	B	401	PEG	C4-C3-O2-C2
6	B	412	NAD	PN-O3-PA-O1A
6	F	402	NAD	PN-O3-PA-O1A
4	B	404	GOL	O1-C1-C2-O2
4	D	405	GOL	O2-C2-C3-O3
3	B	402	PEG	C1-C2-O2-C3
3	A	402	PEG	O1-C1-C2-O2
4	B	405	GOL	O1-C1-C2-O2
3	B	401	PEG	C1-C2-O2-C3
3	B	402	PEG	C4-C3-O2-C2
4	B	409	GOL	O1-C1-C2-O2
4	C	402	GOL	O2-C2-C3-O3
4	H	405	GOL	O2-C2-C3-O3
3	H	401	PEG	O1-C1-C2-O2
3	D	402	PEG	C4-C3-O2-C2
3	A	402	PEG	C4-C3-O2-C2
6	B	412	NAD	PN-O3-PA-O2A
6	F	402	NAD	PN-O3-PA-O2A
6	E	403	NAD	C2D-C1D-N1N-C6N
4	B	408	GOL	O1-C1-C2-O2
6	B	412	NAD	O4D-C1D-N1N-C6N
6	E	403	NAD	O4D-C1D-N1N-C6N
3	B	401	PEG	O1-C1-C2-O2
4	B	405	GOL	O1-C1-C2-C3
6	F	402	NAD	O4B-C4B-C5B-O5B
3	B	402	PEG	O1-C1-C2-O2
6	H	406	NAD	C2B-C1B-N9A-C8A
4	A	403	GOL	O2-C2-C3-O3
3	D	402	PEG	C1-C2-O2-C3
6	G	401	NAD	PN-O3-PA-O2A
6	A	411	NAD	O4B-C4B-C5B-O5B
6	H	406	NAD	O4B-C4B-C5B-O5B

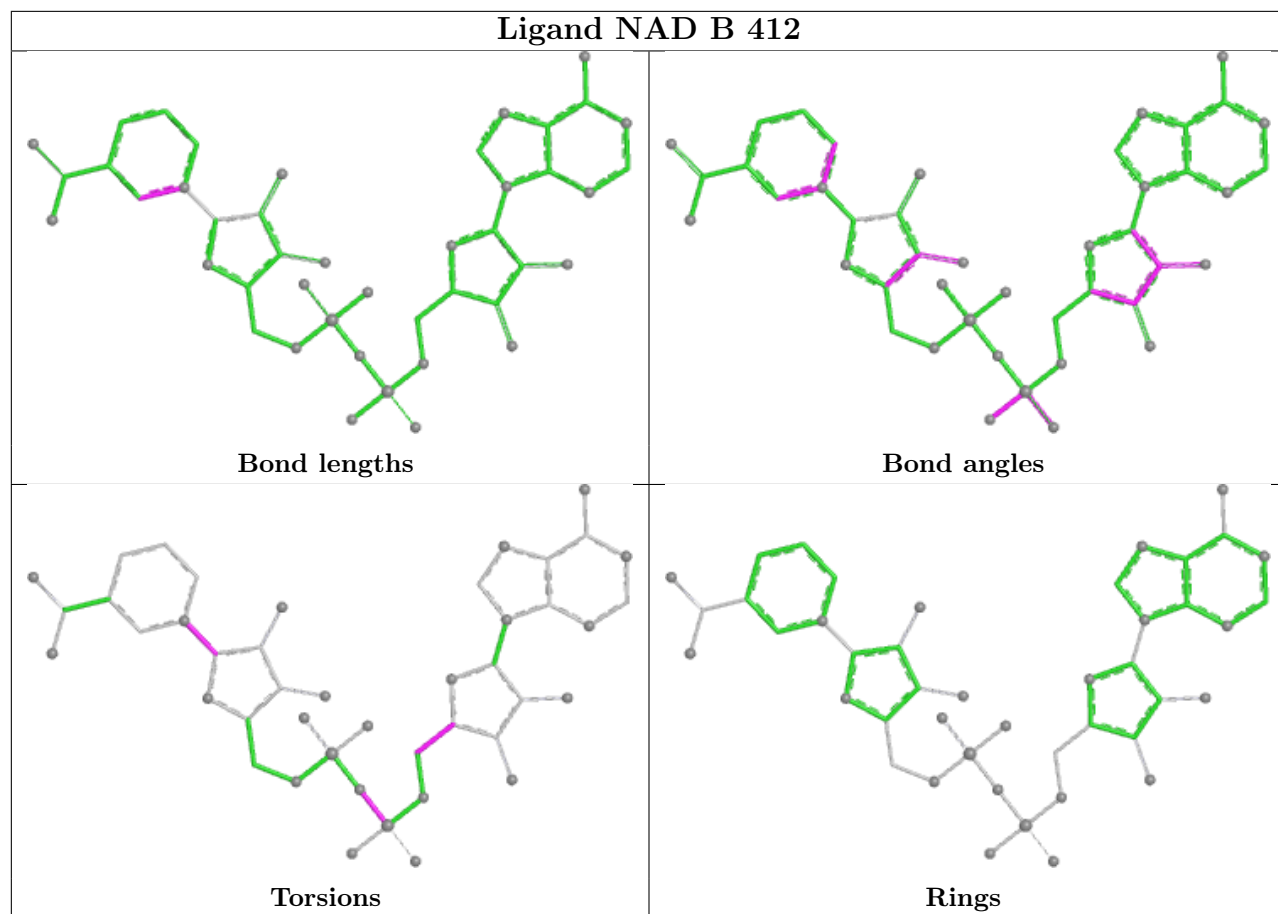
There are no ring outliers.

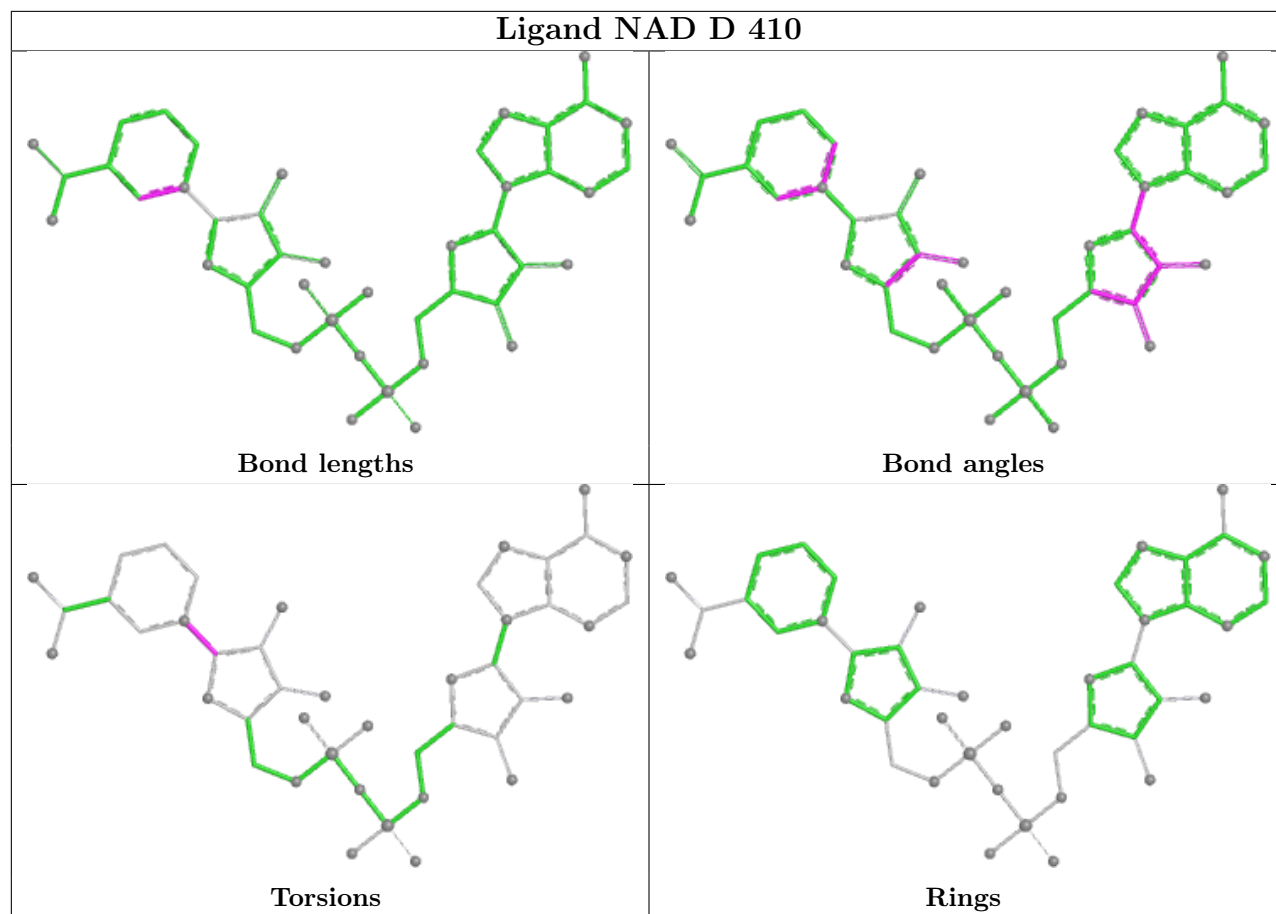
29 monomers are involved in 64 short contacts:

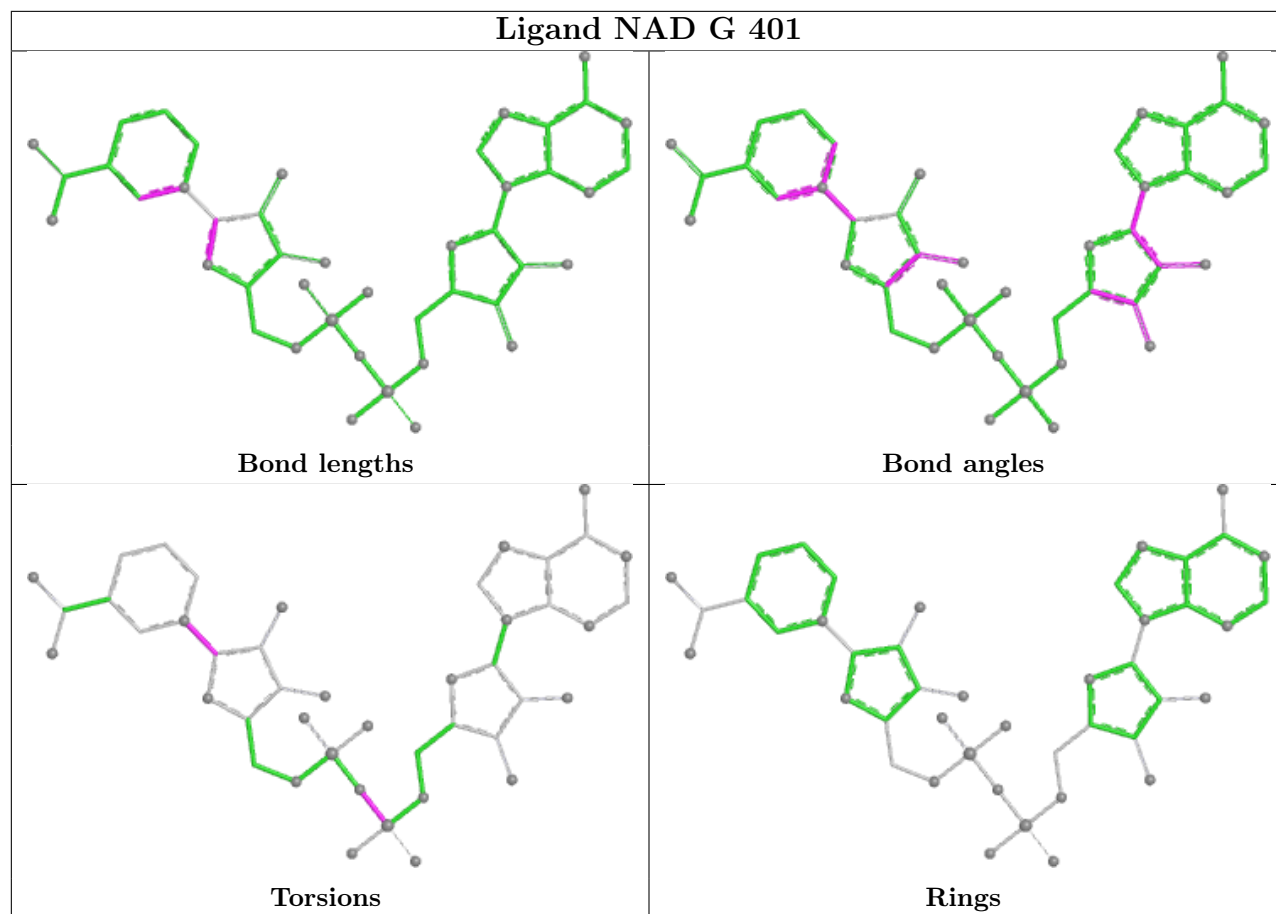
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	PEG	1	0
4	B	409	GOL	4	0
6	H	406	NAD	3	0
4	A	407	GOL	2	0
4	A	406	GOL	1	0
4	B	404	GOL	1	0
6	B	412	NAD	2	0
6	D	410	NAD	2	0
4	D	405	GOL	4	0
4	D	408	GOL	9	0
6	G	401	NAD	1	0
4	B	406	GOL	3	0
4	D	404	GOL	2	0
6	C	405	NAD	2	0
4	C	404	GOL	1	0
3	B	403	PEG	3	0
3	H	401	PEG	1	0
3	A	401	PEG	1	0
4	E	402	GOL	3	0
4	D	401	GOL	1	0
6	E	403	NAD	3	0
4	C	402	GOL	3	0
4	A	412	GOL	3	0
3	A	402	PEG	1	0
4	A	404	GOL	1	0
4	H	403	GOL	6	0
6	A	411	NAD	1	0
6	F	402	NAD	1	0
3	B	402	PEG	4	0

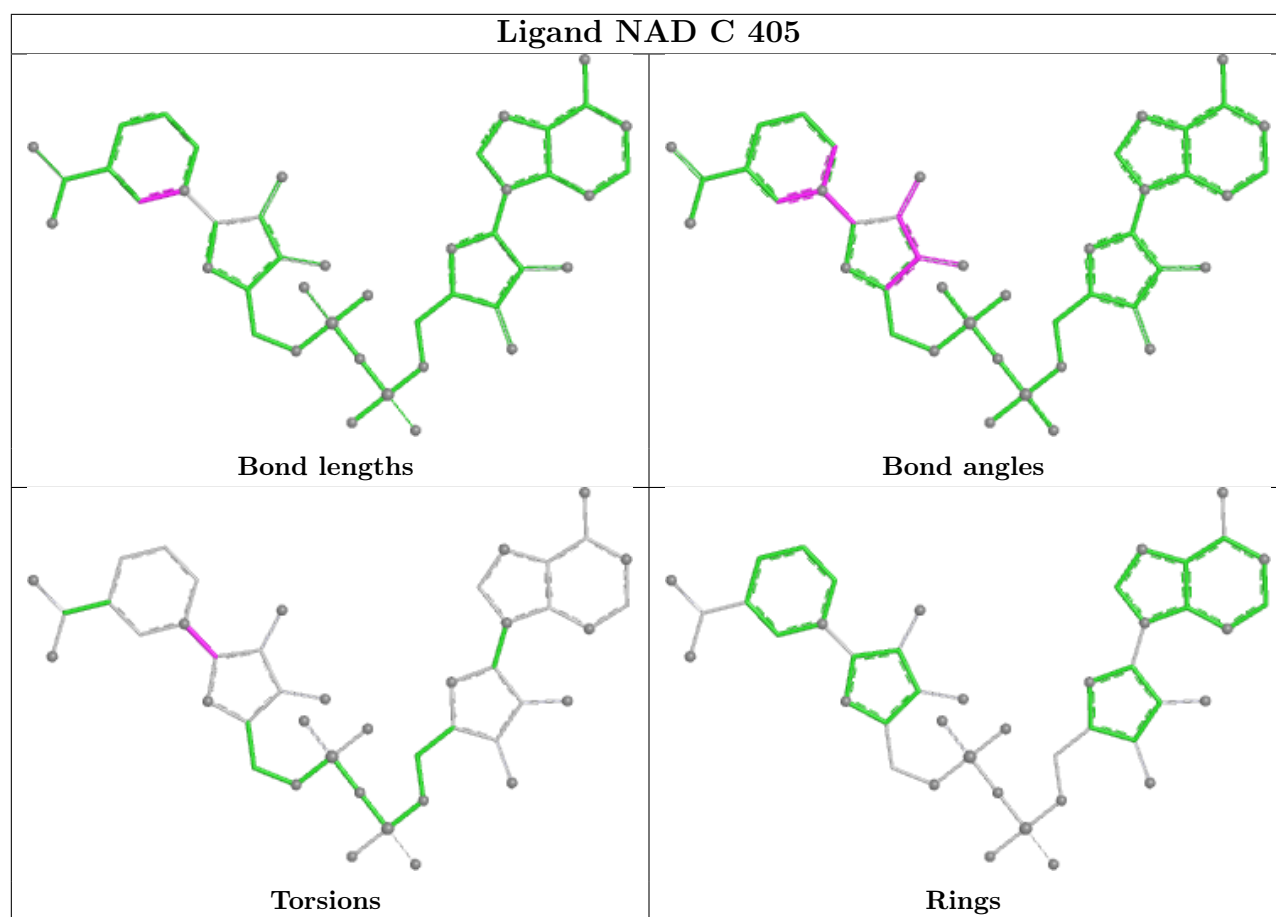
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

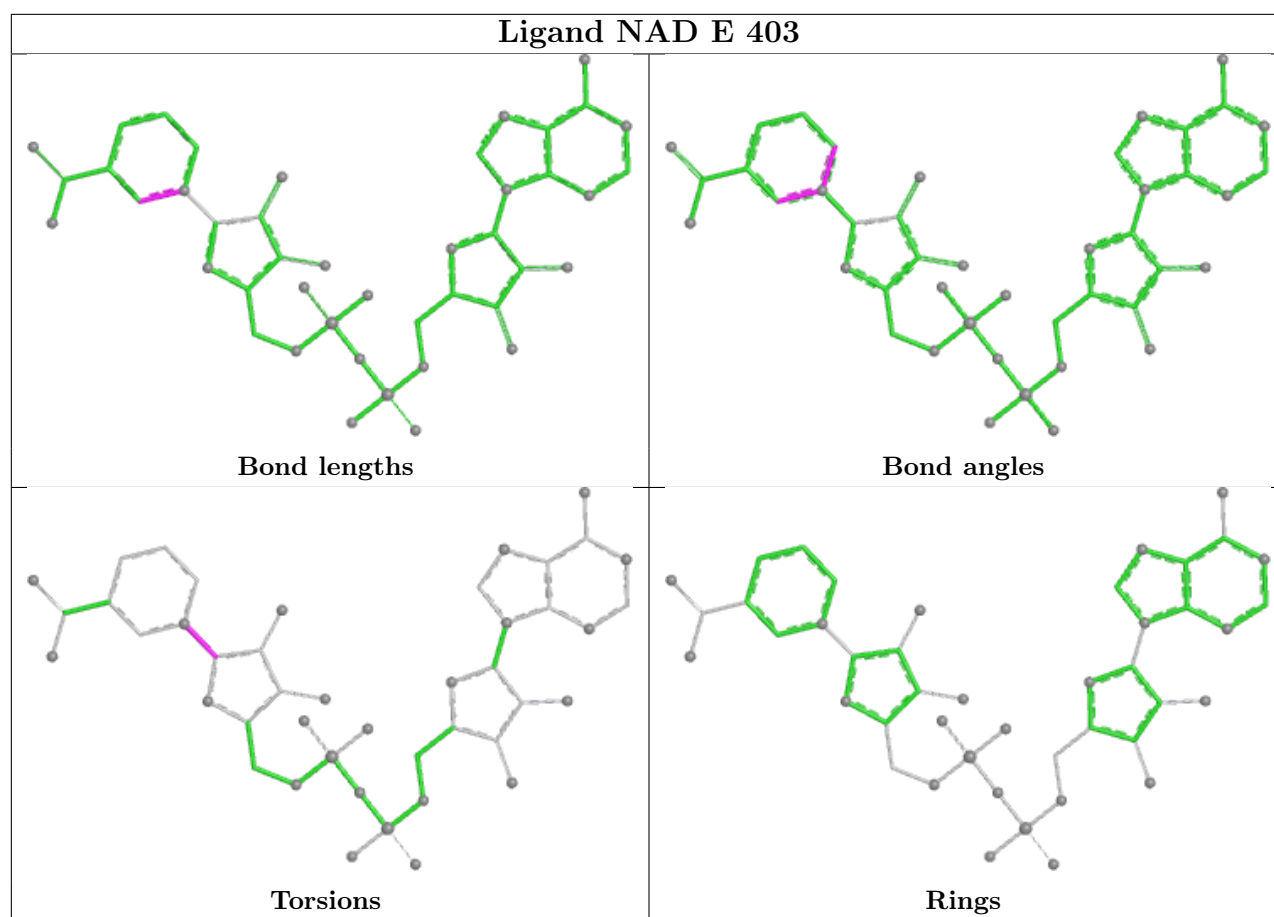


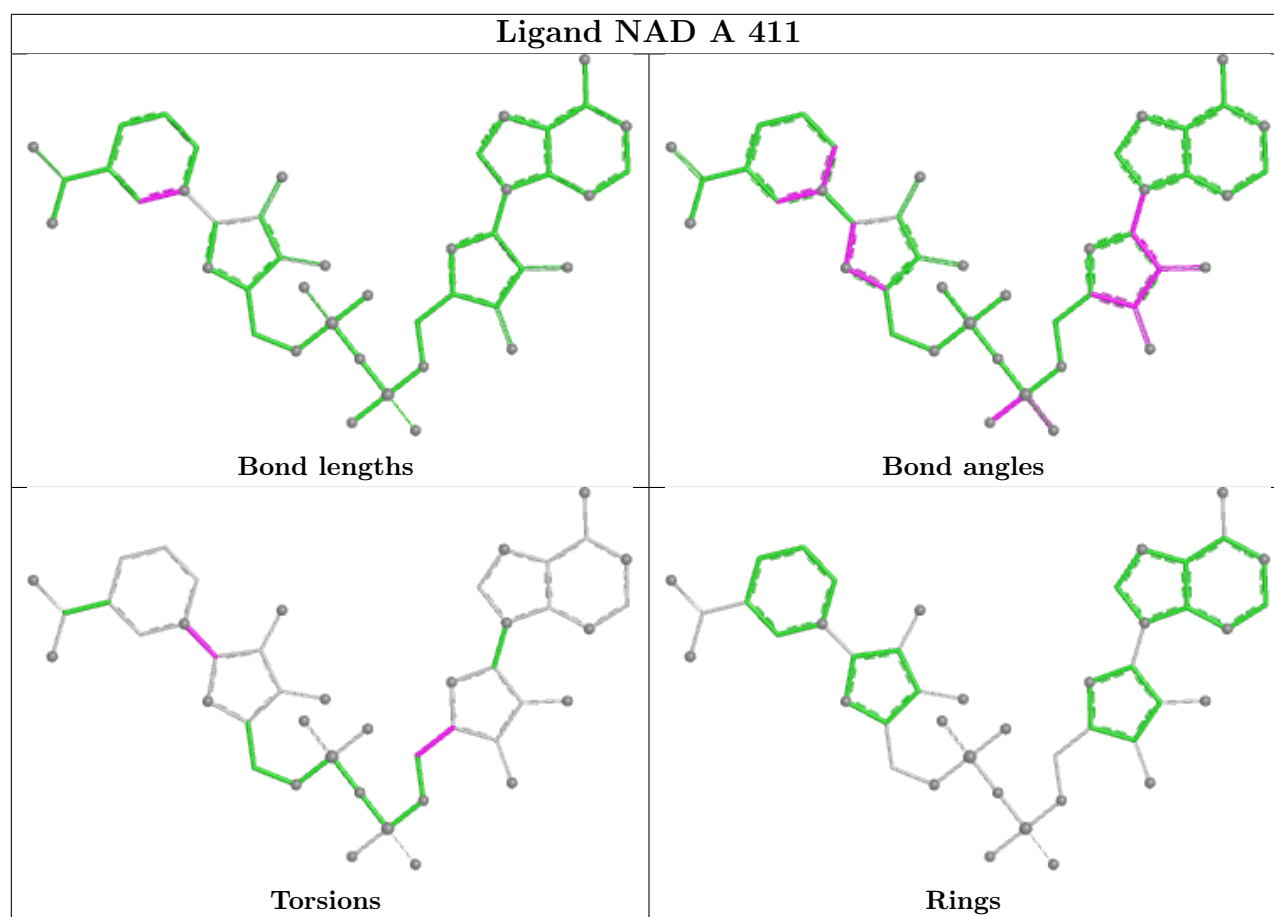


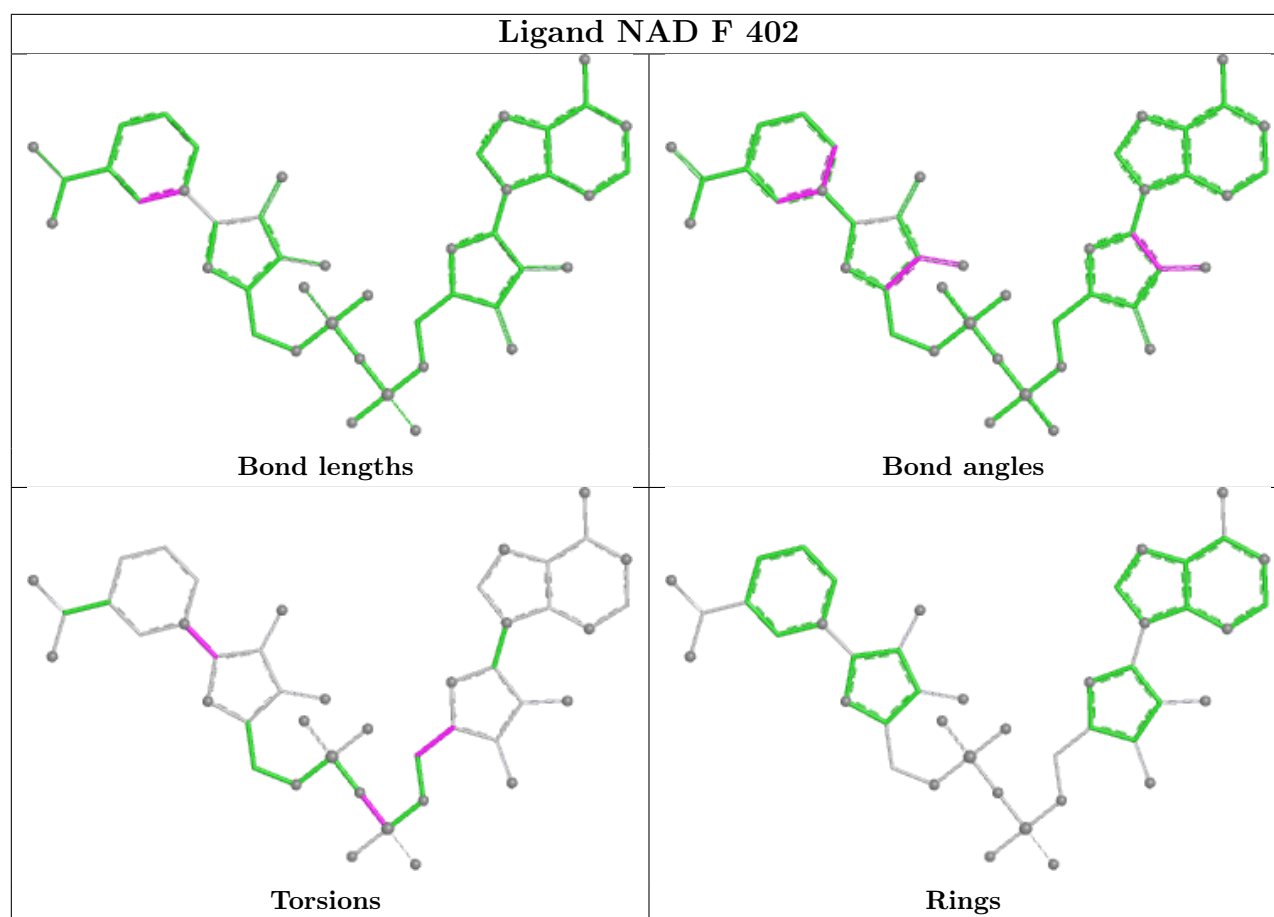












5.7 Other polymers [i](#)

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	333/337 (98%)	0.06	3 (0%) 81 80	36, 50, 81, 108	0
1	B	335/337 (99%)	0.11	5 (1%) 72 71	34, 54, 79, 112	2 (0%)
1	C	333/337 (98%)	0.17	4 (1%) 76 76	36, 56, 86, 115	0
1	D	332/337 (98%)	0.14	2 (0%) 85 85	35, 55, 76, 95	0
1	F	334/337 (99%)	0.33	7 (2%) 63 62	43, 63, 90, 124	0
1	G	333/337 (98%)	0.43	4 (1%) 76 76	46, 67, 92, 115	0
1	H	333/337 (98%)	0.30	6 (1%) 67 66	45, 61, 84, 99	0
2	E	334/337 (99%)	0.28	5 (1%) 72 71	43, 64, 100, 116	0
All	All	2667/2696 (98%)	0.23	36 (1%) 75 74	34, 58, 89, 124	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	214	ALA	3.8
1	B	124[A]	ASP	3.7
1	G	228	LEU	3.5
1	H	0	ALA	3.5
1	B	-1	GLY	3.5
2	E	73	CYS	3.5
1	F	45	LYS	3.1
1	G	307	PHE	2.9
1	F	0	ALA	2.7
1	D	307	PHE	2.6
1	H	307	PHE	2.6
1	B	334	LYS	2.6
1	G	260	ALA	2.5
1	B	69	LYS	2.5
1	A	68	GLY	2.5
1	C	333	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	333	LYS	2.4
1	A	214	ALA	2.3
1	F	63	GLU	2.3
1	B	106	GLU	2.3
1	G	332	ALA	2.3
2	E	113	ALA	2.3
1	H	228	LEU	2.2
1	H	244	ASP	2.2
1	H	210	SER	2.2
1	C	77	ARG	2.2
1	F	184	THR	2.2
1	A	228	LEU	2.1
1	F	106	GLU	2.1
1	F	68	GLY	2.1
1	C	269	ALA	2.1
2	E	126	ASP	2.1
1	F	69	LYS	2.0
2	E	89	VAL	2.0
2	E	61	GLU	2.0
1	D	77	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	B	152	8/9	0.95	0.10	40,46,50,59	0
1	CSD	D	152	8/9	0.96	0.08	43,44,47,57	0
1	CSD	C	152	8/9	0.97	0.07	44,46,50,51	0
1	CSD	A	152	8/9	0.97	0.07	37,43,46,49	0
1	CSD	G	152	8/9	0.97	0.06	52,56,57,58	0
1	CSD	H	152	8/9	0.97	0.06	47,48,50,50	0
1	CSD	F	152	8/9	0.98	0.07	48,48,51,55	0

6.3 Carbohydrates [i](#)

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.

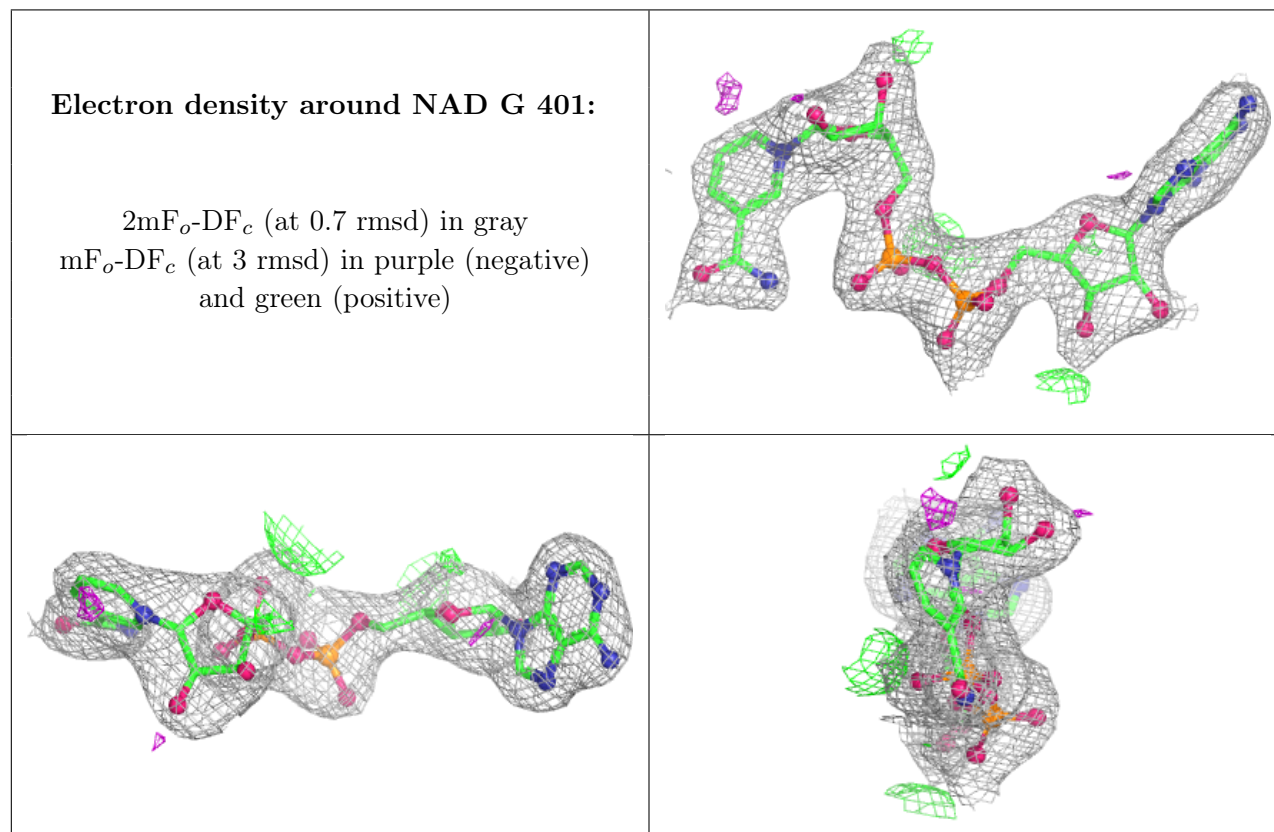
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	E	402	6/6	0.65	0.17	84,85,89,92	0
4	GOL	B	408	6/6	0.72	0.15	64,79,82,86	0
4	GOL	B	407	6/6	0.73	0.17	72,76,81,87	0
3	PEG	H	401	7/7	0.73	0.15	77,77,84,85	0
4	GOL	A	406	6/6	0.73	0.19	57,64,66,67	0
4	GOL	A	408	6/6	0.74	0.12	77,78,81,84	0
4	GOL	B	404	6/6	0.75	0.15	56,63,69,69	0
4	GOL	E	401	6/6	0.77	0.14	63,66,69,70	0
4	GOL	A	409	6/6	0.78	0.12	73,75,77,80	0
4	GOL	H	405	6/6	0.78	0.11	63,66,71,75	0
4	GOL	C	402	6/6	0.80	0.13	57,58,62,63	0
4	GOL	D	407	6/6	0.81	0.12	59,67,70,70	0
3	PEG	B	402	7/7	0.81	0.15	50,53,61,65	0
3	PEG	D	402	7/7	0.81	0.13	66,68,73,77	0
4	GOL	C	403	6/6	0.81	0.12	73,79,80,85	0
5	PO4	B	410	5/5	0.81	0.13	53,54,61,65	5
3	PEG	A	402	7/7	0.82	0.15	57,63,67,70	0
4	GOL	D	405	6/6	0.83	0.14	50,54,57,60	0
4	GOL	C	404	6/6	0.83	0.14	56,59,61,62	0
4	GOL	D	408	6/6	0.84	0.13	56,62,66,68	0
4	GOL	D	404	6/6	0.84	0.14	54,56,59,62	0
3	PEG	B	403	7/7	0.84	0.14	54,58,60,61	0
4	GOL	F	401	6/6	0.84	0.12	72,72,73,78	0
4	GOL	D	406	6/6	0.84	0.12	67,71,74,79	0
4	GOL	A	413	6/6	0.84	0.13	54,60,62,68	0
4	GOL	A	407	6/6	0.85	0.11	60,66,71,72	0
4	GOL	A	412	6/6	0.86	0.11	55,61,66,67	0
4	GOL	D	403	6/6	0.86	0.12	55,58,64,64	0
4	GOL	H	403	6/6	0.86	0.11	55,56,58,62	0
4	GOL	H	404	6/6	0.86	0.13	57,58,60,62	0
4	GOL	B	406	6/6	0.86	0.12	66,67,70,71	0
4	GOL	A	404	6/6	0.86	0.14	55,59,61,62	0
4	GOL	B	405	6/6	0.87	0.12	64,66,69,70	0
4	GOL	A	403	6/6	0.88	0.12	58,62,66,66	0
4	GOL	H	402	6/6	0.88	0.11	67,69,73,75	0
3	PEG	B	401	7/7	0.88	0.12	54,57,60,61	0
5	PO4	D	409	5/5	0.88	0.15	49,51,53,54	5

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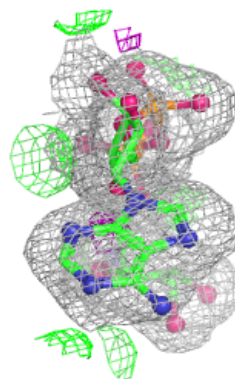
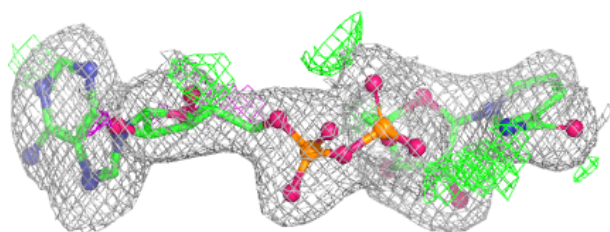
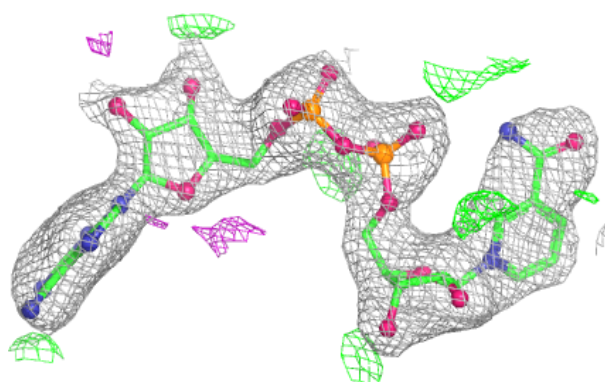
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	B	411	5/5	0.89	0.12	55,58,65,69	5
4	GOL	B	409	6/6	0.89	0.12	57,60,66,67	0
4	GOL	C	401	6/6	0.90	0.11	56,59,61,64	0
3	PEG	A	401	7/7	0.90	0.11	55,56,61,63	0
5	PO4	A	410	5/5	0.92	0.10	47,48,49,53	5
4	GOL	D	401	6/6	0.92	0.10	61,63,68,68	0
6	NAD	G	401	44/44	0.93	0.09	51,57,62,65	0
6	NAD	C	405	44/44	0.94	0.09	45,49,56,63	0
4	GOL	A	405	6/6	0.94	0.10	55,56,57,59	0
6	NAD	E	403	44/44	0.95	0.08	50,58,73,76	0
6	NAD	F	402	44/44	0.95	0.08	44,52,63,64	0
6	NAD	B	412	44/44	0.95	0.08	41,46,53,56	0
6	NAD	A	411	44/44	0.96	0.07	36,45,54,55	0
6	NAD	D	410	44/44	0.97	0.07	37,46,56,65	0
6	NAD	H	406	44/44	0.97	0.07	43,51,56,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

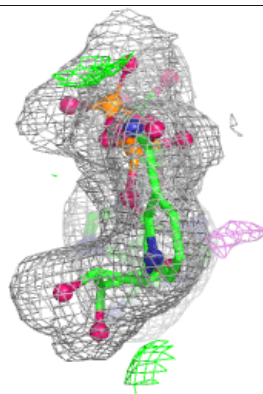
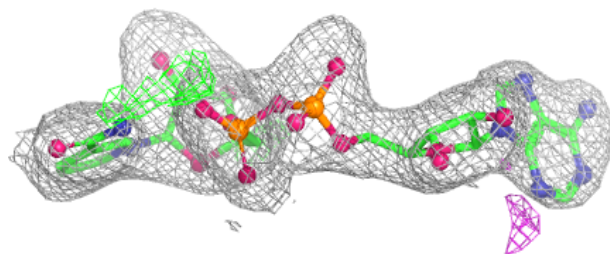
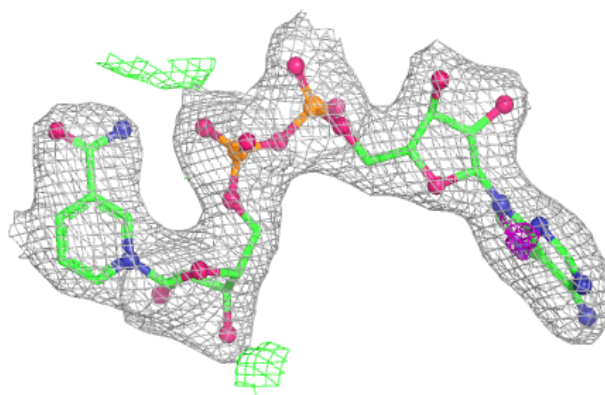


Electron density around NAD C 405:

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

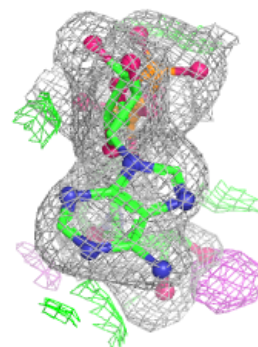
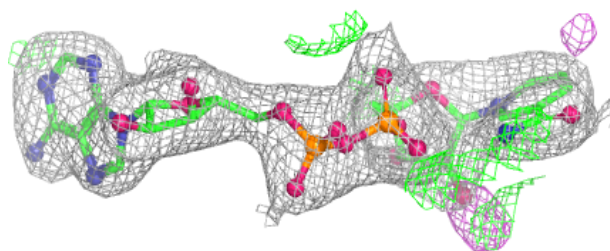
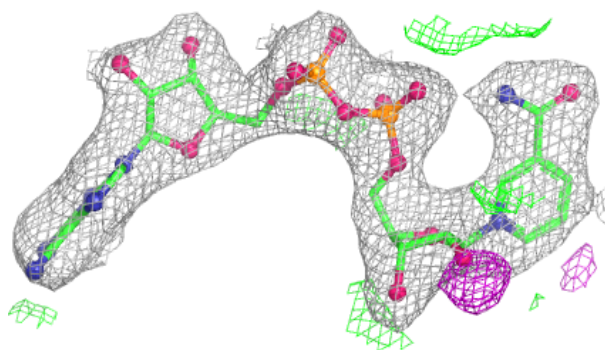
**Electron density around NAD E 403:**

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

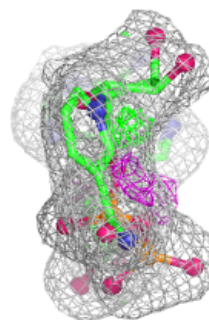
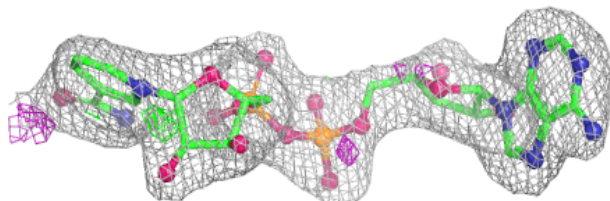
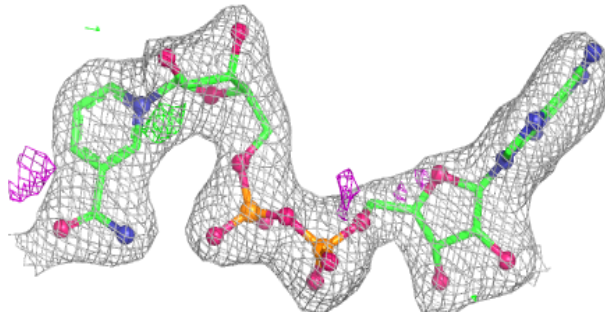


Electron density around NAD F 402:

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

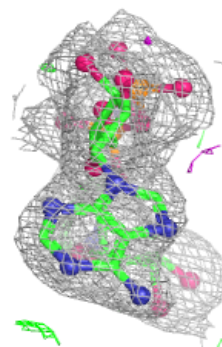
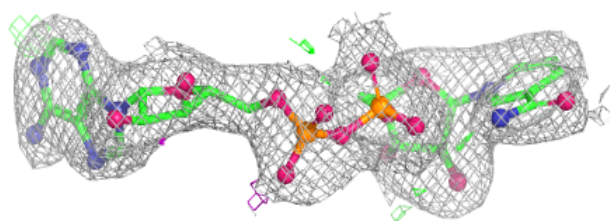
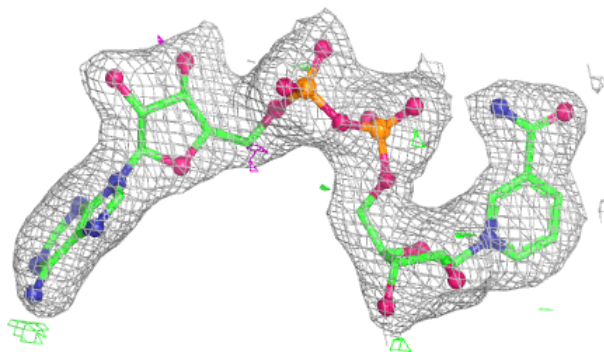
**Electron density around NAD B 412:**

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

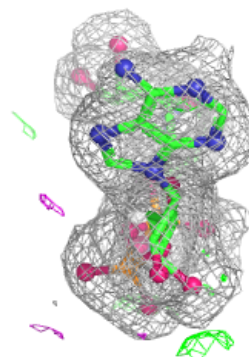
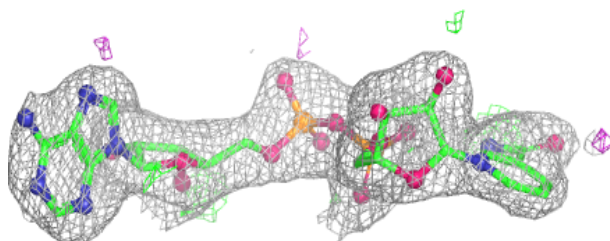
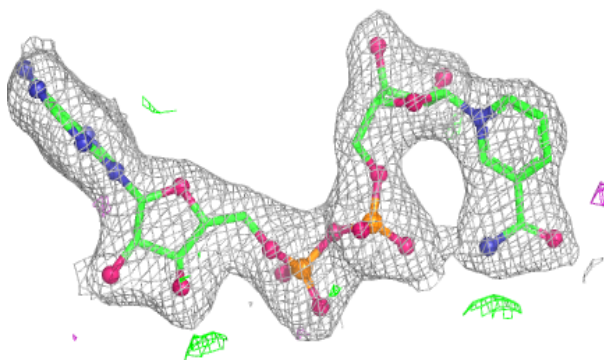


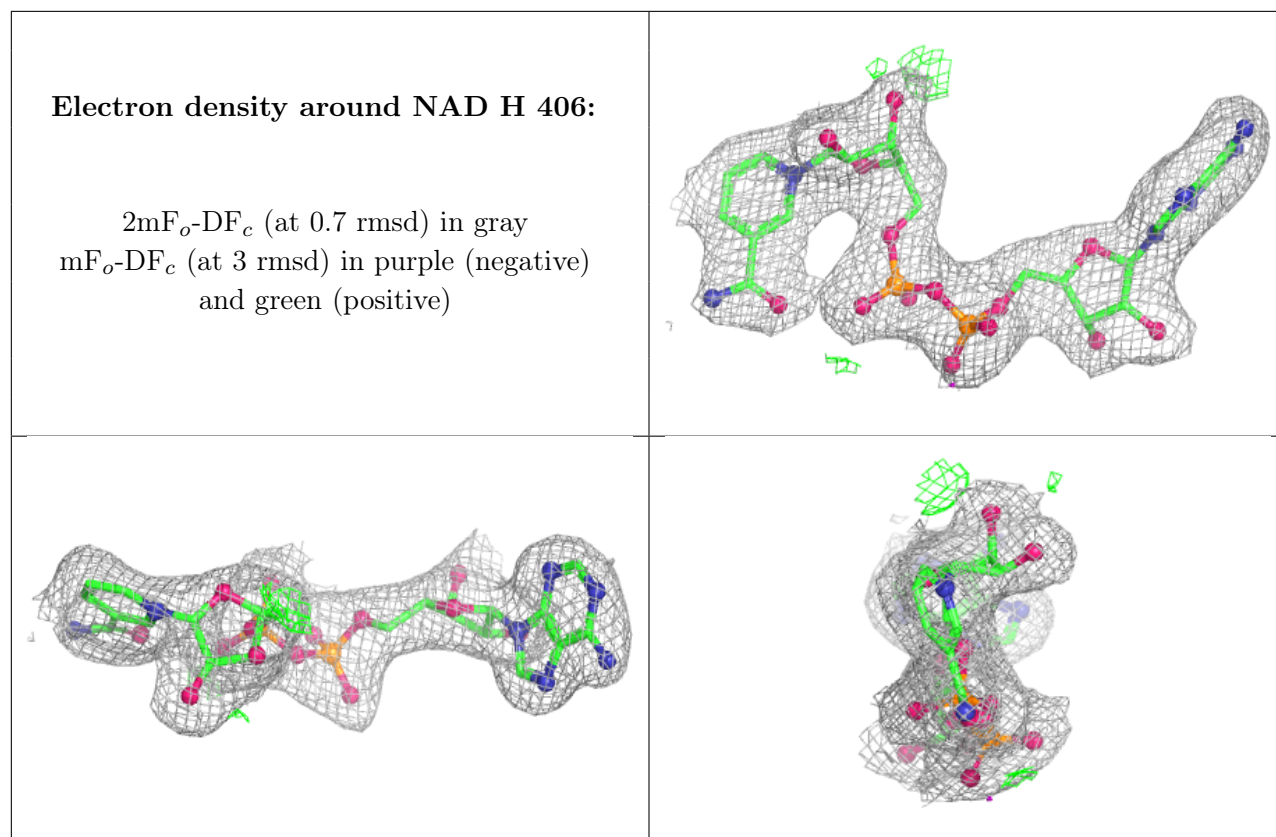
Electron density around NAD A 411:

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

**Electron density around NAD D 410:**

$2mF_o-DF_c$ (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.