



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:42 PM UTC

PDB ID : 1GYQ / pdb_00001gyq
Title : CRYSTAL STRUCTURE OF GLYCOSOMAL GLYCERALDEHYDE FROM
LEISHMANIA MEXICANA IN COMPLEX WITH N6-BENZYL-NAD
Authors : Suresh, S.; Hol, W.
Deposited on : 1999-03-05
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

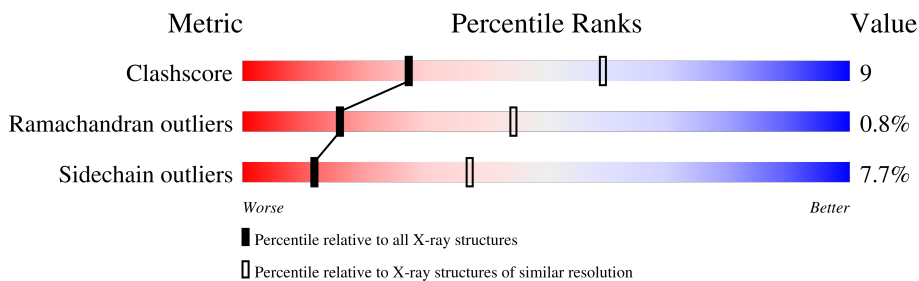
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	358	
1	B	358	
1	C	358	
1	D	358	

2 Entry composition [i](#)

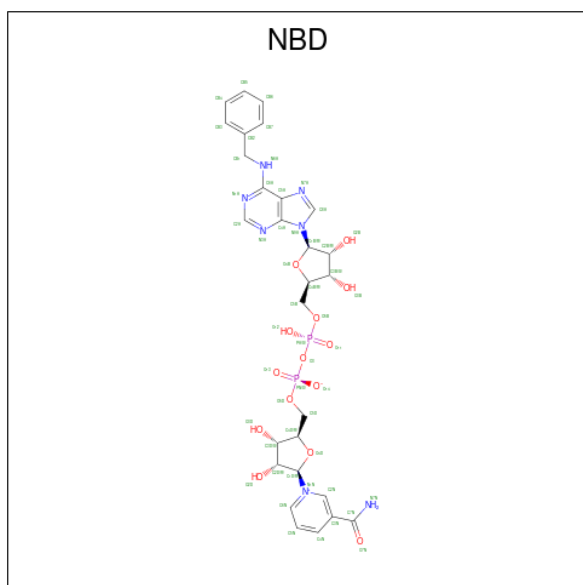
There are 2 unique types of molecules in this entry. The entry contains 11068 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2716	1712	474	517	13			
1	B	358	Total	C	N	O	S	0	0	0
			2716	1712	474	517	13			
1	C	358	Total	C	N	O	S	0	0	0
			2716	1712	474	517	13			
1	D	358	Total	C	N	O	S	0	0	0
			2716	1712	474	517	13			

- Molecule 2 is N6-BENZYL-NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NBD) (formula: C₂₈H₃₃N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			51	28	7	14	2		

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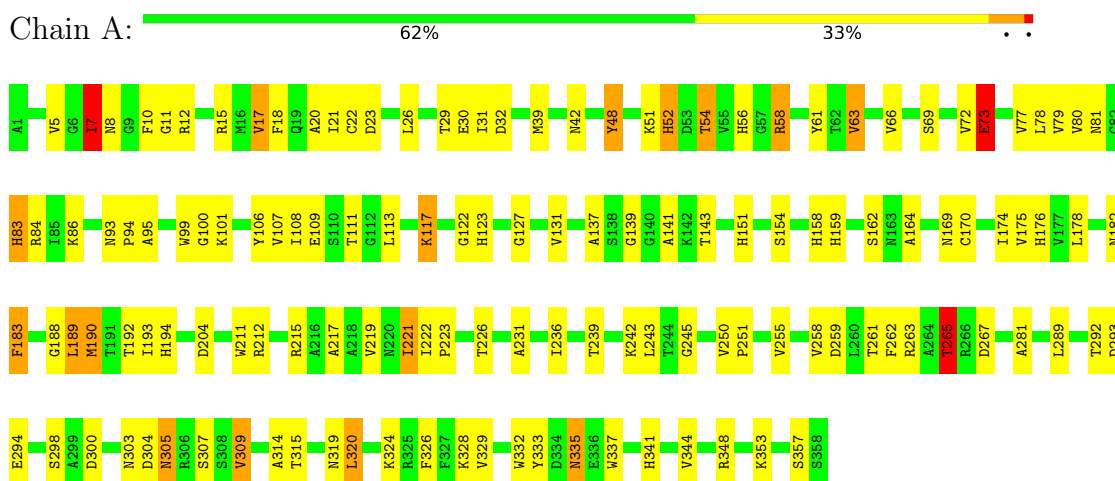
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			51	28	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			51	28	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			51	28	7	14	2		

3 Residue-property plots

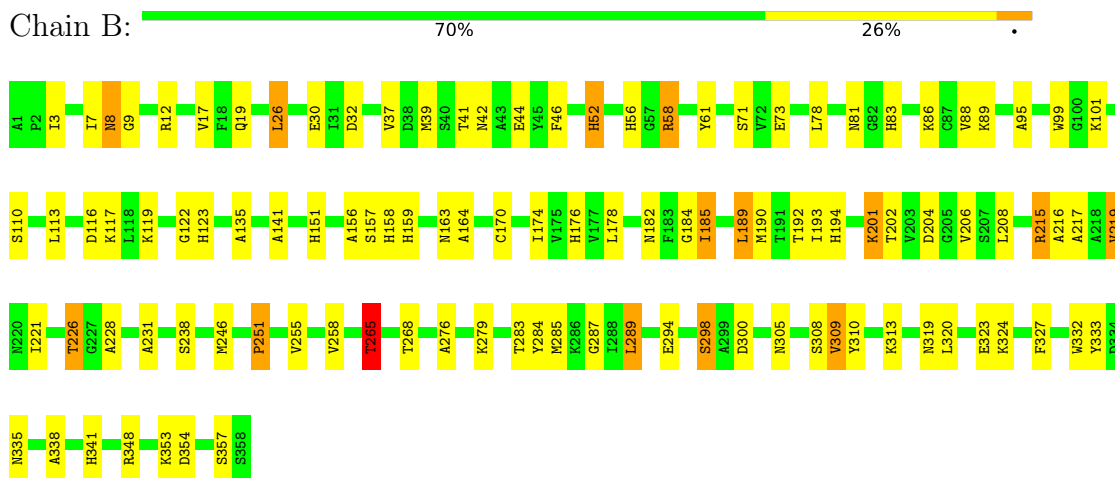
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

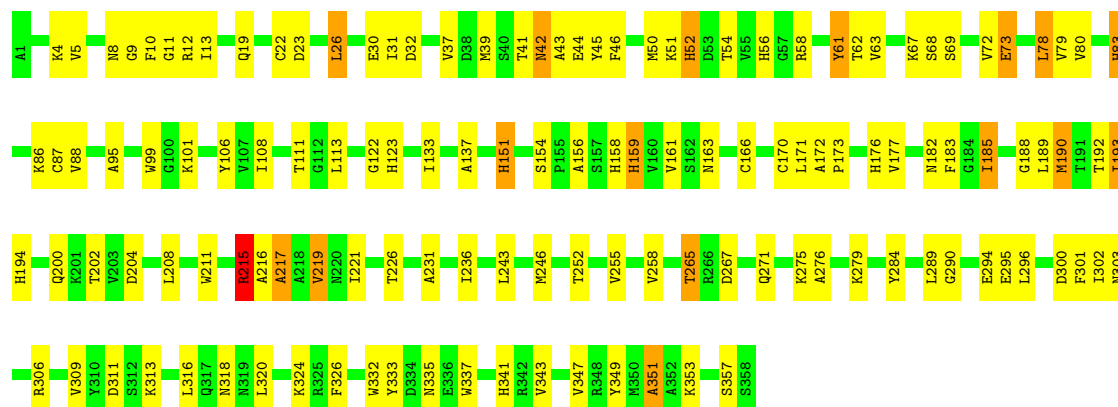


• Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)



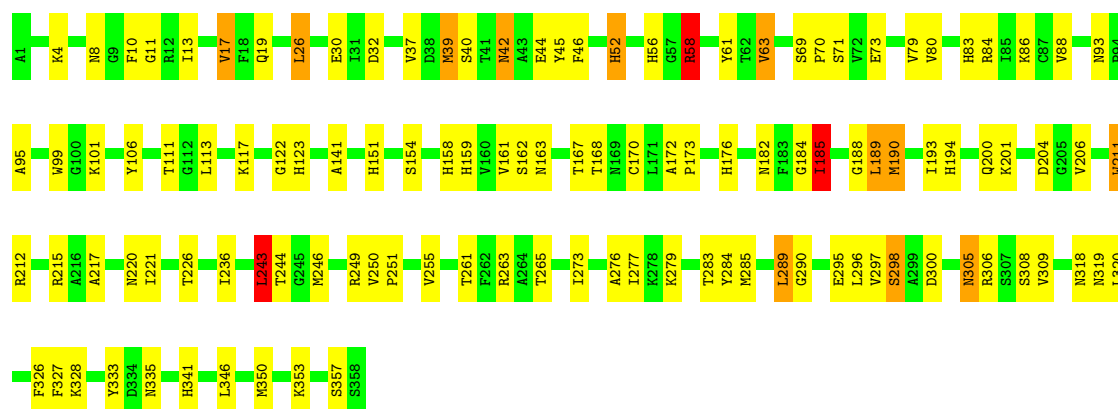
• Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)





- Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

Chain D: 67% 28% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.33Å 125.81Å 137.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.40)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	13.80	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11068	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NBD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	15/2768 (0.5%)	1.79	59/3752 (1.6%)
1	B	1.07	17/2768 (0.6%)	1.76	51/3752 (1.4%)
1	C	0.99	15/2768 (0.5%)	1.75	59/3752 (1.6%)
1	D	1.03	13/2768 (0.5%)	1.71	41/3752 (1.1%)
All	All	1.02	60/11072 (0.5%)	1.75	210/15008 (1.4%)

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

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	ILE	CA-CB	8.16	1.65	1.54
1	B	309	VAL	CA-CB	7.96	1.62	1.53
1	B	341	HIS	CD2-NE2	-7.50	1.29	1.37
1	B	159	HIS	CD2-NE2	-7.48	1.29	1.37
1	B	123	HIS	CD2-NE2	-7.22	1.29	1.37
1	C	52	HIS	CD2-NE2	-6.90	1.30	1.37
1	A	309	VAL	CA-CB	6.89	1.62	1.53
1	A	176	HIS	CD2-NE2	-6.70	1.30	1.37
1	B	151	HIS	CD2-NE2	-6.66	1.30	1.37
1	C	176	HIS	CD2-NE2	-6.65	1.30	1.37
1	D	52	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	52	HIS	CD2-NE2	-6.56	1.30	1.37
1	C	185	ILE	CA-CB	6.54	1.62	1.54
1	C	159	HIS	CD2-NE2	-6.41	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	159	HIS	CD2-NE2	-6.41	1.30	1.37
1	D	176	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	56	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	158	HIS	CD2-NE2	-6.35	1.30	1.37
1	D	123	HIS	CD2-NE2	-6.27	1.30	1.37
1	D	341	HIS	CD2-NE2	-6.26	1.30	1.37
1	C	123	HIS	CD2-NE2	-6.25	1.30	1.37
1	D	83	HIS	CD2-NE2	-6.24	1.30	1.37
1	D	151	HIS	CD2-NE2	-6.20	1.31	1.37
1	B	176	HIS	CD2-NE2	-6.13	1.31	1.37
1	C	194	HIS	CD2-NE2	-6.11	1.31	1.37
1	D	56	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	159	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	83	HIS	CD2-NE2	-6.06	1.31	1.37
1	B	151	HIS	CG-ND1	-6.06	1.31	1.38
1	C	151	HIS	CD2-NE2	-6.05	1.31	1.37
1	B	56	HIS	CG-ND1	-5.99	1.31	1.38
1	B	56	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	52	HIS	CG-ND1	-5.95	1.31	1.38
1	C	56	HIS	CD2-NE2	-5.93	1.31	1.37
1	B	52	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	123	HIS	CD2-NE2	-5.87	1.31	1.37
1	B	341	HIS	CG-ND1	-5.85	1.31	1.38
1	C	83	HIS	CD2-NE2	-5.85	1.31	1.37
1	C	158	HIS	CD2-NE2	-5.80	1.31	1.37
1	D	194	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	341	HIS	CD2-NE2	-5.78	1.31	1.37
1	B	194	HIS	CG-ND1	-5.76	1.31	1.38
1	A	56	HIS	CG-ND1	-5.74	1.31	1.38
1	B	158	HIS	CD2-NE2	-5.73	1.31	1.37
1	B	83	HIS	CD2-NE2	-5.72	1.31	1.37
1	D	158	HIS	CD2-NE2	-5.71	1.31	1.37
1	B	194	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	52	HIS	CG-ND1	-5.60	1.32	1.38
1	C	341	HIS	CD2-NE2	-5.57	1.31	1.37
1	C	194	HIS	CG-ND1	-5.53	1.32	1.38
1	D	151	HIS	CG-ND1	-5.50	1.32	1.38
1	A	151	HIS	CD2-NE2	-5.42	1.31	1.37
1	C	52	HIS	CG-ND1	-5.38	1.32	1.38
1	C	341	HIS	CG-ND1	-5.36	1.32	1.38
1	D	52	HIS	CG-ND1	-5.20	1.32	1.38
1	C	176	HIS	CG-ND1	-5.09	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	185	ILE	CA-CB	5.09	1.60	1.54
1	A	194	HIS	CG-ND1	-5.05	1.32	1.38
1	A	194	HIS	CD2-NE2	-5.02	1.32	1.37
1	A	123	HIS	CG-ND1	-5.01	1.32	1.38

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASN	N-CA-C	10.16	125.07	112.47
1	B	284	TYR	N-CA-C	8.92	123.95	112.89
1	C	284	TYR	N-CA-C	8.85	123.18	112.38
1	B	217	ALA	N-CA-C	8.53	120.66	111.36
1	D	284	TYR	N-CA-C	8.42	123.37	113.18
1	D	32	ASP	CA-CB-CG	8.39	120.99	112.60
1	C	182	ASN	N-CA-C	8.36	123.17	113.38
1	A	217	ALA	N-CA-C	8.11	120.11	111.28
1	B	26	LEU	N-CA-C	7.97	122.11	112.38
1	B	32	ASP	CA-CB-CG	7.90	120.50	112.60
1	A	221	ILE	N-CA-C	-7.82	95.86	107.51
1	B	283	THR	CA-C-O	-7.59	114.29	119.68
1	D	182	ASN	N-CA-C	7.59	121.84	112.58
1	C	23	ASP	CA-CB-CG	7.52	120.12	112.60
1	B	185	ILE	CA-C-O	7.45	126.85	120.22
1	C	193	ILE	N-CA-C	-7.44	96.84	108.23
1	B	8	ASN	CA-CB-CG	7.42	120.02	112.60
1	B	219	VAL	N-CA-CB	-7.36	99.08	111.23
1	D	217	ALA	N-CA-C	7.36	121.50	112.23
1	A	304	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	193	ILE	N-CA-C	-7.28	96.38	107.73
1	A	259	ASP	CA-CB-CG	7.15	119.75	112.60
1	D	42	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	B	156	ALA	N-CA-C	6.92	118.82	111.28
1	B	231	ALA	N-CA-C	6.87	120.54	111.75
1	D	327	PHE	N-CA-C	6.85	120.57	109.40
1	A	305	ASN	N-CA-C	6.83	120.58	112.93
1	C	303	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	C	231	ALA	N-CA-C	6.80	119.53	111.71
1	B	338	ALA	CA-C-O	-6.78	113.91	120.90
1	D	163	ASN	CA-CB-CG	6.77	119.37	112.60
1	C	217	ALA	N-CA-C	6.71	120.69	112.23
1	A	337	TRP	N-CA-C	6.71	118.38	111.14
1	D	193	ILE	N-CA-C	-6.70	98.62	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASN	CA-CB-CG	6.66	119.25	112.60
1	C	335	ASN	CB-CG-ND2	6.64	126.37	116.40
1	C	252	THR	CA-C-N	6.63	126.22	119.19
1	C	252	THR	C-N-CA	6.63	126.22	119.19
1	A	23	ASP	CA-CB-CG	6.63	119.23	112.60
1	D	221	ILE	N-CA-C	-6.61	99.06	108.58
1	C	320	LEU	CA-C-N	6.56	126.06	119.24
1	C	320	LEU	C-N-CA	6.56	126.06	119.24
1	A	217	ALA	O-C-N	6.55	129.06	122.12
1	D	17	VAL	N-CA-C	-6.52	104.40	110.53
1	C	219	VAL	N-CA-CB	-6.50	100.50	111.23
1	A	99	TRP	CG-CD2-CE3	6.45	140.35	133.90
1	B	221	ILE	N-CA-C	-6.43	98.60	107.99
1	D	318	ASN	N-CA-C	6.40	119.75	112.97
1	C	341	HIS	CA-C-O	-6.38	114.13	120.70
1	C	99	TRP	CG-CD2-CE3	6.33	140.23	133.90
1	A	183	PHE	N-CA-C	-6.33	104.31	111.14
1	D	99	TRP	N-CA-C	6.25	118.61	111.11
1	A	192	THR	CA-CB-OG1	-6.24	100.24	109.60
1	B	208	LEU	N-CA-C	6.23	119.05	111.82
1	B	332	TRP	CG-CD2-CE3	6.19	140.09	133.90
1	B	265	THR	CA-CB-OG1	-6.19	100.32	109.60
1	D	159	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	B	182	ASN	N-CA-C	6.14	120.06	112.58
1	C	154	SER	CA-C-N	6.12	125.80	119.56
1	C	154	SER	C-N-CA	6.12	125.80	119.56
1	A	42	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	D	8	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	C	302	ILE	O-C-N	6.06	129.63	122.66
1	B	354	ASP	CA-CB-CG	6.04	118.64	112.60
1	D	93	ASN	CA-C-N	6.03	127.38	119.84
1	D	93	ASN	C-N-CA	6.03	127.38	119.84
1	B	251	PRO	N-CA-C	6.03	124.89	112.47
1	C	32	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	313	LYS	CA-CB-CG	-5.99	102.13	114.10
1	C	68	SER	N-CA-C	5.97	117.79	111.28
1	A	176	HIS	CB-CG-CD2	-5.94	123.47	131.20
1	C	163	ASN	CB-CG-ND2	5.94	125.31	116.40
1	C	301	PHE	CA-CB-CG	-5.90	107.90	113.80
1	D	357	SER	CA-C-N	5.89	132.30	121.70
1	D	357	SER	C-N-CA	5.89	132.30	121.70
1	A	10	PHE	N-CA-CB	-5.89	103.35	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	A	222	ILE	CA-C-O	-5.85	114.81	119.25
1	A	29	THR	N-CA-C	5.84	119.59	112.23
1	B	310	TYR	N-CA-C	5.84	118.95	110.42
1	C	123	HIS	CA-CB-CG	-5.82	107.98	113.80
1	C	8	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	B	287	GLY	CA-C-N	5.80	128.65	122.97
1	B	287	GLY	C-N-CA	5.80	128.65	122.97
1	C	357	SER	CA-C-N	5.79	132.12	121.70
1	C	357	SER	C-N-CA	5.79	132.12	121.70
1	A	265	THR	CA-CB-OG1	-5.75	100.97	109.60
1	D	26	LEU	N-CA-C	5.75	120.29	113.28
1	A	341	HIS	CA-CB-CG	-5.74	108.06	113.80
1	A	194	HIS	CA-CB-CG	5.72	119.52	113.80
1	A	305	ASN	CA-CB-CG	5.70	118.30	112.60
1	A	293	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	123	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	A	51	LYS	CB-CG-CD	-5.69	98.22	111.30
1	B	338	ALA	N-CA-C	-5.69	104.72	111.03
1	A	222	ILE	N-CA-CB	-5.65	104.65	111.31
1	C	341	HIS	N-CA-C	-5.65	105.04	111.14
1	C	41	THR	N-CA-C	-5.64	107.03	114.31
1	D	58	ARG	N-CA-C	-5.64	102.93	109.93
1	D	194	HIS	CB-CG-CD2	-5.64	123.86	131.20
1	B	159	HIS	CA-CB-CG	-5.63	108.17	113.80
1	D	123	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	A	22	CYS	N-CA-C	5.62	117.09	111.07
1	B	81	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	303	ASN	N-CA-C	5.61	120.07	113.23
1	A	7	ILE	CA-CB-CG2	-5.60	100.98	110.50
1	D	251	PRO	N-CA-C	5.56	123.49	113.70
1	A	251	PRO	N-CA-C	5.55	123.90	112.47
1	A	31	ILE	CA-C-O	5.55	126.48	120.43
1	A	320	LEU	CA-C-N	5.55	125.21	119.05
1	A	320	LEU	C-N-CA	5.55	125.21	119.05
1	D	319	ASN	CA-CB-CG	-5.54	107.06	112.60
1	D	305	ASN	N-CA-C	5.53	119.66	113.02
1	C	163	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	D	283	THR	CA-C-O	-5.53	116.18	119.55
1	B	193	ILE	N-CA-C	-5.52	100.37	108.54
1	A	123	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	C	161	VAL	N-CA-CB	-5.51	105.49	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	TYR	N-CA-C	-5.49	105.38	111.36
1	B	192	THR	CA-CB-OG1	-5.49	101.37	109.60
1	C	351	ALA	N-CA-C	5.48	118.01	111.71
1	D	8	ASN	CB-CG-ND2	5.47	124.61	116.40
1	C	215	ARG	NE-CZ-NH1	5.46	126.97	121.50
1	C	236	ILE	CA-C-N	5.46	125.13	119.56
1	C	236	ILE	C-N-CA	5.46	125.13	119.56
1	B	332	TRP	CE2-CD2-CG	-5.46	100.65	107.20
1	D	39	MET	N-CA-C	5.45	117.92	111.33
1	C	133	ILE	N-CA-CB	5.45	117.21	111.00
1	B	348	ARG	CA-CB-CG	-5.44	103.22	114.10
1	D	99	TRP	CG-CD2-CE3	5.44	139.34	133.90
1	B	313	LYS	CA-C-O	-5.43	115.10	120.70
1	C	316	LEU	N-CA-C	5.43	117.28	111.36
1	B	357	SER	CA-C-N	5.42	131.46	121.70
1	B	357	SER	C-N-CA	5.42	131.46	121.70
1	C	137	ALA	N-CA-C	5.42	118.30	109.24
1	C	159	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	D	201	LYS	N-CA-C	5.42	118.23	109.40
1	A	357	SER	CA-C-N	5.40	131.42	121.70
1	A	357	SER	C-N-CA	5.40	131.42	121.70
1	C	337	TRP	N-CA-C	5.39	116.97	111.14
1	C	311	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	99	TRP	CB-CG-CD1	-5.39	118.82	126.90
1	B	332	TRP	CB-CG-CD1	-5.38	118.83	126.90
1	A	281	ALA	N-CA-C	5.37	118.05	111.82
1	C	172	ALA	CA-C-N	5.37	124.82	119.24
1	C	172	ALA	C-N-CA	5.37	124.82	119.24
1	C	133	ILE	CB-CA-C	-5.37	104.47	110.96
1	D	168	THR	N-CA-C	-5.37	105.34	111.14
1	A	226	THR	CA-CB-OG1	-5.35	101.58	109.60
1	B	163	ASN	CB-CG-ND2	5.33	124.40	116.40
1	D	236	ILE	CA-C-N	5.33	125.00	119.56
1	D	236	ILE	C-N-CA	5.33	125.00	119.56
1	C	332	TRP	CE2-CD2-CG	-5.32	100.82	107.20
1	A	73	GLU	N-CA-C	5.32	117.16	111.36
1	C	176	HIS	CB-CG-CD2	-5.31	124.29	131.20
1	D	176	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	C	61	TYR	N-CA-C	5.31	117.39	110.43
1	C	192	THR	CA-CB-OG1	-5.31	101.64	109.60
1	C	318	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	B	99	TRP	CE2-CD2-CG	-5.30	100.84	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	C	123	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	C	318	ASN	N-CA-C	5.30	119.05	112.59
1	B	17	VAL	N-CA-C	-5.28	105.35	110.42
1	C	69	SER	O-C-N	-5.28	117.26	121.80
1	B	159	HIS	N-CA-C	5.25	119.68	113.12
1	A	99	TRP	CE2-CD2-CG	-5.24	100.92	107.20
1	A	21	ILE	CA-C-O	-5.23	115.69	121.29
1	A	154	SER	CA-C-N	5.23	125.54	119.47
1	A	154	SER	C-N-CA	5.23	125.54	119.47
1	A	231	ALA	N-CA-C	5.23	118.44	111.75
1	A	236	ILE	CA-C-N	5.21	124.87	119.56
1	A	236	ILE	C-N-CA	5.21	124.87	119.56
1	C	159	HIS	CA-CB-CG	-5.20	108.60	113.80
1	A	211	TRP	CG-CD2-CE3	5.20	139.10	133.90
1	A	332	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	C	99	TRP	CB-CG-CD1	-5.20	119.10	126.90
1	C	341	HIS	CA-CB-CG	-5.20	108.60	113.80
1	A	17	VAL	N-CA-C	-5.19	105.48	110.72
1	A	93	ASN	CA-C-N	5.19	126.33	119.84
1	A	93	ASN	C-N-CA	5.19	126.33	119.84
1	D	243	LEU	N-CA-CB	-5.18	101.63	111.00
1	B	110	SER	N-CA-C	5.17	117.07	110.61
1	B	323	GLU	N-CA-C	5.17	117.93	110.28
1	B	226	THR	N-CA-CB	-5.17	102.58	110.85
1	D	99	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	B	219	VAL	CB-CA-C	5.12	119.69	111.29
1	B	3	ILE	N-CA-C	-5.10	101.24	108.58
1	D	206	VAL	N-CA-C	5.09	116.08	108.54
1	A	32	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	22	CYS	N-CA-C	5.07	116.89	111.36
1	D	158	HIS	N-CA-C	5.07	116.58	108.41
1	A	292	THR	O-C-N	5.06	129.46	123.33
1	B	320	LEU	CA-C-N	5.06	124.85	119.28
1	B	320	LEU	C-N-CA	5.06	124.85	119.28
1	D	154	SER	CA-C-N	5.06	124.84	119.28
1	D	154	SER	C-N-CA	5.06	124.84	119.28
1	B	202	THR	O-C-N	5.06	127.92	122.15
1	B	327	PHE	N-CA-C	5.05	117.83	109.85
1	C	335	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	56	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	C	42	ASN	OD1-CG-ND2	-5.04	117.56	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	PRO	N-CA-CB	5.03	107.79	103.31
1	A	159	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	D	211	TRP	CG-CD2-CE3	5.03	138.93	133.90
1	A	326	PHE	N-CA-C	5.02	116.78	108.20
1	B	135	ALA	CA-C-N	5.01	124.93	119.76
1	B	135	ALA	C-N-CA	5.01	124.93	119.76
1	C	313	LYS	CA-CB-CG	-5.00	104.09	114.10
1	C	332	TRP	CG-CD1-NE1	-5.00	103.70	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	215	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	2716	0	2736	73	0
1	B	2716	0	2736	47	0
1	C	2716	0	2736	63	0
1	D	2716	0	2736	63	0
2	A	51	0	32	10	0
2	B	51	0	32	5	0
2	C	51	0	32	7	0
2	D	51	0	32	9	0
All	All	11068	0	11072	201	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 9.

All (201) 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:39:MET:HE1	2:D:361:NBD:CB5	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:MET:HE2	1:C:226:THR:HG21	1.61	0.82
1:C:113:LEU:HD12	2:C:361:NBD:HB11	1.65	0.77
1:A:39:MET:HE1	2:A:361:NBD:CB5	2.19	0.72
1:B:116:ASP:HB3	1:B:119:LYS:HG3	1.72	0.71
1:A:111:THR:HG22	2:A:361:NBD:N3A	2.07	0.69
1:D:190:MET:HE2	1:D:226:THR:HG21	1.73	0.69
1:D:113:LEU:HD12	2:D:361:NBD:HB11	1.76	0.67
1:D:113:LEU:CD1	2:D:361:NBD:HB11	2.24	0.67
1:A:190:MET:HG3	1:A:245:GLY:HA3	1.76	0.66
1:A:63:VAL:HG13	1:A:80:VAL:HG22	1.77	0.66
1:A:5:VAL:HG12	1:A:106:TYR:HB2	1.77	0.65
1:D:117:LYS:HB2	1:D:141:ALA:HB2	1.79	0.64
1:D:111:THR:HG22	2:D:361:NBD:N3A	2.12	0.64
1:B:39:MET:HE1	2:B:361:NBD:CB5	2.28	0.63
1:A:169:ASN:O	1:A:307:SER:HB3	1.98	0.63
1:D:37:VAL:HG22	1:D:88:VAL:HB	1.79	0.63
1:A:7:ILE:HD13	1:A:108:ILE:HD12	1.79	0.63
1:D:200:GLN:OE1	1:D:249:ARG:HD2	2.00	0.61
1:C:204:ASP:OD1	1:C:215:ARG:HD2	2.00	0.61
1:A:111:THR:HG22	2:A:361:NBD:C2A	2.32	0.60
1:A:328:LYS:HB2	1:D:189:LEU:HD23	1.84	0.60
1:C:290:GLY:HA3	1:C:306:ARG:NH1	2.15	0.60
1:C:5:VAL:HG12	1:C:106:TYR:HB2	1.84	0.60
1:B:184:GLY:HA3	1:B:265:THR:HB	1.83	0.60
1:B:41:THR:HG23	1:B:89:LYS:HE2	1.83	0.60
1:B:298:SER:HB3	1:C:221:ILE:H	1.68	0.59
1:B:335:ASN:O	2:B:361:NBD:H4N	2.02	0.59
1:A:315:THR:HG23	1:A:328:LYS:O	2.02	0.59
1:C:208:LEU:HD11	1:D:40:SER:HB2	1.85	0.59
1:C:10:PHE:CD2	1:C:46:PHE:HD2	2.21	0.57
1:A:189:LEU:HD23	1:D:328:LYS:HB2	1.85	0.57
1:D:190:MET:CE	1:D:226:THR:HG21	2.35	0.57
1:C:52:HIS:HB3	1:D:215:ARG:NH2	2.20	0.57
1:D:188:GLY:O	1:D:243:LEU:HA	2.05	0.56
1:A:267:ASP:HB3	1:A:324:LYS:HD2	1.87	0.56
1:C:37:VAL:HG22	1:C:88:VAL:HB	1.88	0.56
1:A:215:ARG:NH2	1:D:300:ASP:OD1	2.35	0.56
1:A:183:PHE:O	1:A:265:THR:HB	2.06	0.55
1:C:95:ALA:HA	1:C:122:GLY:O	2.07	0.55
1:A:212:ARG:HG2	1:D:295:GLU:HB3	1.87	0.55
1:A:212:ARG:HD3	1:D:296:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HG23	1:A:77:VAL:HB	1.88	0.55
1:A:320:LEU:HG	1:D:244:THR:HG22	1.88	0.55
1:D:111:THR:HG22	2:D:361:NBD:C2A	2.36	0.55
1:A:258:VAL:HG23	1:A:333:TYR:CE1	2.42	0.54
1:B:42:ASN:HD21	1:B:44:GLU:HB2	1.72	0.54
1:A:261:THR:HG21	1:D:261:THR:HB	1.90	0.54
1:A:212:ARG:HB3	1:D:297:VAL:CG1	2.37	0.54
1:B:19:GLN:HG3	1:B:61:TYR:HE2	1.72	0.54
1:C:267:ASP:HB3	1:C:324:LYS:HD2	1.90	0.54
1:D:79:VAL:HG22	1:D:84:ARG:HG2	1.89	0.53
1:C:43:ALA:HB1	1:C:78:LEU:HD13	1.91	0.53
1:C:258:VAL:HG23	1:C:333:TYR:HE1	1.74	0.53
1:A:61:TYR:HE1	1:A:63:VAL:HG22	1.75	0.52
1:A:95:ALA:HA	1:A:122:GLY:O	2.10	0.52
1:B:190:MET:HE3	1:B:226:THR:HG21	1.91	0.52
1:B:190:MET:HE1	1:B:228:ALA:HB3	1.92	0.52
1:C:113:LEU:CD1	2:C:361:NBD:HB11	2.38	0.52
1:A:188:GLY:HA2	1:D:326:PHE:CE1	2.45	0.52
1:A:242:LYS:O	1:D:320:LEU:HD11	2.10	0.52
1:A:258:VAL:HG23	1:A:333:TYR:HE1	1.75	0.52
1:C:9:GLY:HA2	2:C:361:NBD:N3A	2.25	0.52
1:A:61:TYR:CE1	1:A:63:VAL:HG22	2.45	0.51
1:B:258:VAL:HG23	1:B:333:TYR:HE1	1.76	0.51
1:A:69:SER:O	1:A:72:VAL:HG22	2.10	0.51
1:B:258:VAL:HG23	1:B:333:TYR:CE1	2.45	0.51
1:A:250:VAL:HG11	1:D:250:VAL:HG11	1.91	0.51
1:B:204:ASP:OD2	1:B:215:ARG:HD2	2.11	0.51
1:A:117:LYS:HG2	1:A:139:GLY:O	2.10	0.51
1:C:39:MET:HE1	2:C:361:NBD:CB5	2.40	0.51
1:A:18:PHE:CZ	1:A:80:VAL:HG21	2.46	0.50
1:A:52:HIS:HE1	1:C:294:GLU:OE1	1.92	0.50
1:A:262:PHE:HE1	1:A:329:VAL:HG23	1.77	0.50
1:A:175:VAL:HG11	1:A:239:THR:HG21	1.94	0.50
1:C:11:GLY:HA3	2:C:361:NBD:O5B	2.11	0.50
1:A:8:ASN:ND2	2:A:361:NBD:H2A	2.27	0.50
1:B:189:LEU:HD22	1:C:326:PHE:HD1	1.76	0.49
1:A:12:ARG:HH11	1:B:204:ASP:HB2	1.76	0.49
1:D:111:THR:CG2	2:D:361:NBD:C2A	2.91	0.49
1:A:300:ASP:OD2	1:D:215:ARG:NH2	2.46	0.49
1:C:108:ILE:HD11	1:C:347:VAL:HG21	1.95	0.49
1:C:111:THR:HG22	2:C:361:NBD:C2A	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:CD1	2:A:361:NBD:HB11	2.42	0.49
1:A:107:VAL:HB	1:A:131:VAL:HG22	1.95	0.48
1:D:113:LEU:HD12	2:D:361:NBD:CB1	2.43	0.48
1:C:19:GLN:HG3	1:C:61:TYR:CE2	2.49	0.48
1:A:111:THR:CG2	2:A:361:NBD:C2A	2.91	0.48
1:B:189:LEU:HB2	1:C:326:PHE:HE1	1.79	0.48
1:C:211:TRP:CE2	1:D:45:TYR:HD1	2.32	0.48
1:A:294:GLU:OE1	1:C:52:HIS:HE1	1.97	0.47
1:B:95:ALA:HA	1:B:122:GLY:O	2.14	0.47
1:C:62:THR:O	1:C:80:VAL:HA	2.14	0.47
1:C:26:LEU:HB3	1:C:31:ILE:HB	1.96	0.47
1:C:43:ALA:HA	1:C:46:PHE:HD1	1.78	0.47
1:D:170:CYS:HA	1:D:308:SER:HB2	1.96	0.47
1:A:79:VAL:HG22	1:A:84:ARG:HG2	1.97	0.47
1:C:73:GLU:H	1:C:73:GLU:CD	2.23	0.47
1:B:276:ALA:HA	1:B:279:LYS:HE2	1.97	0.47
1:C:13:ILE:HG13	2:C:361:NBD:C2N	2.45	0.46
1:B:19:GLN:HG3	1:B:61:TYR:CE2	2.50	0.46
1:B:113:LEU:HD12	2:B:361:NBD:HB11	1.97	0.46
1:B:117:LYS:HB2	1:B:141:ALA:HB2	1.97	0.46
1:A:52:HIS:HD2	1:A:58:ARG:NH1	2.13	0.46
1:C:78:LEU:HD22	1:C:87:CYS:SG	2.55	0.46
1:C:79:VAL:HA	1:C:83:HIS:O	2.15	0.46
1:B:8:ASN:HA	1:B:37:VAL:HB	1.96	0.46
1:B:268:THR:O	1:B:324:LYS:HA	2.15	0.46
1:A:12:ARG:NH1	1:B:204:ASP:HB2	2.30	0.46
1:D:10:PHE:HD2	1:D:46:PHE:HD2	1.64	0.46
1:D:10:PHE:CD2	1:D:46:PHE:HD2	2.33	0.46
1:A:17:VAL:HG11	1:A:108:ILE:HD13	1.98	0.46
1:C:42:ASN:HD21	1:C:44:GLU:HB2	1.79	0.46
1:A:188:GLY:O	1:A:243:LEU:HA	2.16	0.46
1:D:276:ALA:HA	1:D:279:LYS:HE2	1.98	0.46
1:B:285:MET:HB3	1:B:289:LEU:HB2	1.98	0.45
1:D:290:GLY:HA3	1:D:306:ARG:NH1	2.32	0.45
1:A:52:HIS:CE1	1:C:296:LEU:HD21	2.51	0.45
1:B:42:ASN:ND2	1:B:44:GLU:HB2	2.32	0.45
1:C:188:GLY:O	1:C:243:LEU:HA	2.17	0.45
1:A:52:HIS:HD2	1:A:58:ARG:HH11	1.65	0.45
1:B:9:GLY:HA2	2:B:361:NBD:N3A	2.32	0.45
1:C:19:GLN:HG3	1:C:61:TYR:HE2	1.83	0.44
1:D:273:ILE:O	1:D:277:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:HIS:HA	1:C:349:TYR:OH	2.17	0.44
1:A:11:GLY:O	1:A:15:ARG:HG3	2.18	0.44
1:A:314:ALA:HB2	1:D:212:ARG:NH2	2.32	0.44
1:C:171:LEU:HD22	1:C:190:MET:SD	2.57	0.44
1:C:170:CYS:SG	1:C:333:TYR:CD1	3.09	0.43
1:D:19:GLN:HG3	1:D:61:TYR:HE2	1.83	0.43
1:A:215:ARG:NH2	1:D:300:ASP:CG	2.77	0.43
1:C:258:VAL:HG23	1:C:333:TYR:CE1	2.53	0.43
1:A:204:ASP:HB2	1:B:12:ARG:NH1	2.33	0.43
1:C:193:ILE:HD12	1:C:193:ILE:N	2.33	0.43
1:B:300:ASP:OD2	1:C:215:ARG:NH2	2.51	0.43
1:C:183:PHE:O	1:C:265:THR:HB	2.19	0.43
1:A:335:ASN:O	2:A:361:NBD:H4N	2.19	0.43
1:D:42:ASN:HD21	1:D:44:GLU:HB2	1.83	0.43
1:B:300:ASP:O	1:D:58:ARG:NH2	2.51	0.43
1:A:170:CYS:SG	1:A:333:TYR:CD1	3.12	0.43
1:B:300:ASP:OD1	1:C:215:ARG:NH2	2.48	0.43
1:A:39:MET:HE1	2:A:361:NBD:CB6	2.49	0.42
1:B:42:ASN:O	1:B:46:PHE:HD1	2.02	0.42
1:C:12:ARG:HH11	1:D:204:ASP:HB2	1.84	0.42
1:D:346:LEU:O	1:D:350:MET:HG3	2.18	0.42
1:B:246:MET:HE3	1:B:246:MET:HB2	1.90	0.42
1:C:200:GLN:HB3	1:C:217:ALA:HB2	2.00	0.42
1:C:276:ALA:HA	1:C:279:LYS:HE2	2.01	0.42
1:D:13:ILE:O	1:D:17:VAL:HG23	2.19	0.42
1:A:221:ILE:H	1:D:298:SER:HB3	1.85	0.42
1:A:54:THR:HG21	1:B:216:ALA:HB3	2.02	0.42
1:A:113:LEU:HD12	2:A:361:NBD:HB11	2.01	0.42
1:C:271:GLN:O	1:C:275:LYS:HG3	2.20	0.42
1:B:174:ILE:O	1:B:178:LEU:HG	2.20	0.42
1:C:5:VAL:HA	1:C:106:TYR:O	2.19	0.42
1:A:48:TYR:CE1	1:C:295:GLU:HB2	2.55	0.41
1:B:215:ARG:NH2	1:C:300:ASP:OD2	2.52	0.41
1:B:294:GLU:OE2	1:D:52:HIS:HE1	2.03	0.41
1:C:54:THR:HB	1:D:204:ASP:OD1	2.20	0.41
1:D:285:MET:HB3	1:D:289:LEU:HB2	2.02	0.41
1:A:54:THR:HB	1:B:204:ASP:OD1	2.20	0.41
1:A:73:GLU:CD	1:A:73:GLU:H	2.28	0.41
1:B:37:VAL:HG22	1:B:88:VAL:HB	2.02	0.41
1:B:113:LEU:CD1	2:B:361:NBD:HB11	2.50	0.41
1:D:95:ALA:HA	1:D:122:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HA	1:A:83:HIS:O	2.19	0.41
1:A:174:ILE:O	1:A:178:LEU:HG	2.20	0.41
1:B:42:ASN:ND2	1:B:44:GLU:H	2.18	0.41
1:C:156:ALA:O	1:C:159:HIS:HE1	2.03	0.41
1:B:170:CYS:HA	1:B:308:SER:HB2	2.01	0.41
1:A:100:GLY:H	1:A:127:GLY:HA3	1.85	0.41
1:D:63:VAL:HG13	1:D:80:VAL:HG22	2.02	0.41
1:D:246:MET:HE3	1:D:246:MET:HB2	1.88	0.41
1:D:161:VAL:HG21	1:D:350:MET:SD	2.61	0.41
1:A:137:ALA:HB3	1:A:141:ALA:HB3	2.03	0.41
1:A:143:THR:HA	1:A:162:SER:O	2.21	0.41
1:C:46:PHE:O	1:C:50:MET:SD	2.79	0.41
1:C:106:TYR:OH	1:C:351:ALA:HA	2.20	0.41
1:C:215:ARG:O	1:C:216:ALA:C	2.63	0.41
1:C:246:MET:HE3	1:C:246:MET:HB2	1.92	0.41
1:D:11:GLY:HA3	2:D:361:NBD:O5B	2.21	0.41
1:D:39:MET:HE1	2:D:361:NBD:CB4	2.46	0.41
1:C:12:ARG:NH1	1:D:204:ASP:HB2	2.36	0.41
1:C:67:LYS:HB3	1:C:72:VAL:CG2	2.51	0.41
1:D:106:TYR:CD1	1:D:106:TYR:N	2.89	0.41
1:D:172:ALA:HB3	1:D:173:PRO:HD3	2.03	0.40
1:A:263:ARG:HD2	1:D:263:ARG:HD2	2.02	0.40
1:A:298:SER:OG	1:D:220:ASN:HA	2.20	0.40
1:A:20:ALA:HB3	1:A:344:VAL:HG21	2.04	0.40
1:C:45:TYR:HD1	1:D:211:TRP:CE2	2.39	0.40
1:A:204:ASP:HB2	1:B:12:ARG:HH11	1.87	0.40
1:B:189:LEU:HB2	1:C:326:PHE:CE1	2.56	0.40
1:B:201:LYS:HE3	1:B:206:VAL:O	2.22	0.40
1:D:42:ASN:ND2	1:D:44:GLU:H	2.19	0.40
1:D:185:ILE:HD11	1:D:243:LEU:HB2	2.02	0.40
1:A:111:THR:HG22	2:A:361:NBD:C4A	2.50	0.40
1:A:215:ARG:NH2	1:B:52:HIS:HB3	2.37	0.40
1:A:300:ASP:CG	1:D:215:ARG:HH22	2.28	0.40
1:B:52:HIS:HD2	1:B:58:ARG:NH1	2.19	0.40
1:C:42:ASN:ND2	1:C:44:GLU:HB2	2.37	0.40
1:D:170:CYS:SG	1:D:333:TYR:CD1	3.15	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/358 (99%)	325 (91%)	27 (8%)	4 (1%)	11	38
1	B	356/358 (99%)	333 (94%)	20 (6%)	3 (1%)	16	44
1	C	356/358 (99%)	330 (93%)	25 (7%)	1 (0%)	36	65
1	D	356/358 (99%)	332 (93%)	21 (6%)	3 (1%)	16	44
All	All	1424/1432 (99%)	1320 (93%)	93 (6%)	11 (1%)	16	44

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	VAL
1	B	255	VAL
1	C	255	VAL
1	D	70	PRO
1	D	184	GLY
1	D	255	VAL
1	A	117	LYS
1	A	164	ALA
1	B	164	ALA
1	A	219	VAL
1	B	251	PRO

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	294/294 (100%)	272 (92%)	22 (8%)	12	38
1	B	294/294 (100%)	271 (92%)	23 (8%)	11	37
1	C	294/294 (100%)	271 (92%)	23 (8%)	11	37
1	D	294/294 (100%)	271 (92%)	23 (8%)	11	37
All	All	1176/1176 (100%)	1085 (92%)	91 (8%)	12	37

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	26	LEU
1	A	30	GLU
1	A	54	THR
1	A	58	ARG
1	A	63	VAL
1	A	73	GLU
1	A	78	LEU
1	A	86	LYS
1	A	94	PRO
1	A	101	LYS
1	A	109	GLU
1	A	189	LEU
1	A	190	MET
1	A	265	THR
1	A	289	LEU
1	A	305	ASN
1	A	309	VAL
1	A	319	ASN
1	A	335	ASN
1	A	348	ARG
1	A	353	LYS
1	B	7	ILE
1	B	26	LEU
1	B	30	GLU
1	B	58	ARG
1	B	71	SER
1	B	73	GLU
1	B	78	LEU
1	B	86	LYS
1	B	101	LYS
1	B	157	SER
1	B	185	ILE

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Mol	Chain	Res	Type
1	B	189	LEU
1	B	201	LYS
1	B	215	ARG
1	B	219	VAL
1	B	238	SER
1	B	265	THR
1	B	289	LEU
1	B	298	SER
1	B	305	ASN
1	B	309	VAL
1	B	319	ASN
1	B	353	LYS
1	C	4	LYS
1	C	26	LEU
1	C	30	GLU
1	C	51	LYS
1	C	58	ARG
1	C	63	VAL
1	C	73	GLU
1	C	78	LEU
1	C	86	LYS
1	C	101	LYS
1	C	166	CYS
1	C	173	PRO
1	C	177	VAL
1	C	185	ILE
1	C	189	LEU
1	C	190	MET
1	C	202	THR
1	C	219	VAL
1	C	265	THR
1	C	289	LEU
1	C	309	VAL
1	C	343	VAL
1	C	353	LYS
1	D	4	LYS
1	D	26	LEU
1	D	30	GLU
1	D	58	ARG
1	D	63	VAL
1	D	69	SER
1	D	71	SER

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Mol	Chain	Res	Type
1	D	73	GLU
1	D	86	LYS
1	D	101	LYS
1	D	162	SER
1	D	167	THR
1	D	185	ILE
1	D	189	LEU
1	D	190	MET
1	D	243	LEU
1	D	265	THR
1	D	289	LEU
1	D	298	SER
1	D	305	ASN
1	D	309	VAL
1	D	335	ASN
1	D	353	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	19	GLN
1	A	42	ASN
1	A	52	HIS
1	A	91	GLN
1	A	159	HIS
1	A	305	ASN
1	B	42	ASN
1	B	49	GLN
1	B	52	HIS
1	B	151	HIS
1	B	159	HIS
1	B	305	ASN
1	B	341	HIS
1	C	42	ASN
1	C	52	HIS
1	C	151	HIS
1	C	159	HIS
1	C	318	ASN
1	C	341	HIS
1	D	8	ASN
1	D	24	GLN

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Mol	Chain	Res	Type
1	D	42	ASN
1	D	52	HIS
1	D	305	ASN
1	D	341	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NBD	C	361	-	54,56,56	1.58	11 (20%)	74,83,83	1.62	16 (21%)
2	NBD	D	361	-	54,56,56	1.59	11 (20%)	74,83,83	1.62	16 (21%)
2	NBD	B	361	-	54,56,56	1.58	11 (20%)	74,83,83	1.63	16 (21%)
2	NBD	A	361	-	54,56,56	1.58	11 (20%)	74,83,83	1.62	16 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NBD	C	361	-	-	11/35/67/67	0/6/6/6
2	NBD	D	361	-	-	11/35/67/67	0/6/6/6
2	NBD	B	361	-	-	11/35/67/67	0/6/6/6
2	NBD	A	361	-	-	11/35/67/67	0/6/6/6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	361	NBD	C2N-N1N	6.66	1.42	1.35
2	B	361	NBD	C2N-N1N	6.60	1.42	1.35
2	A	361	NBD	C2N-N1N	6.60	1.42	1.35
2	C	361	NBD	C2N-N1N	6.55	1.42	1.35
2	C	361	NBD	CB3-CB2	2.80	1.44	1.38
2	B	361	NBD	CB3-CB2	2.79	1.44	1.38
2	D	361	NBD	CB3-CB2	2.78	1.44	1.38
2	A	361	NBD	CB3-CB2	2.78	1.44	1.38
2	C	361	NBD	O4D-C1D	2.75	1.44	1.40
2	A	361	NBD	O4D-C1D	2.73	1.44	1.40
2	D	361	NBD	O4D-C1D	2.73	1.44	1.40
2	B	361	NBD	O4D-C1D	2.72	1.44	1.40
2	D	361	NBD	CB4-CB3	2.63	1.43	1.38
2	D	361	NBD	C5A-N7A	-2.62	1.34	1.39
2	A	361	NBD	C5A-N7A	-2.62	1.34	1.39
2	D	361	NBD	CB6-CB7	2.62	1.43	1.38
2	C	361	NBD	CB6-CB7	2.61	1.43	1.38
2	A	361	NBD	CB4-CB3	2.60	1.43	1.38
2	A	361	NBD	CB6-CB7	2.60	1.43	1.38
2	B	361	NBD	CB6-CB7	2.60	1.43	1.38
2	B	361	NBD	CB4-CB3	2.60	1.43	1.38
2	C	361	NBD	CB4-CB3	2.59	1.43	1.38
2	C	361	NBD	CB7-CB2	2.59	1.44	1.38
2	B	361	NBD	C5A-N7A	-2.58	1.34	1.39
2	B	361	NBD	CB7-CB2	2.58	1.44	1.38
2	C	361	NBD	C5A-N7A	-2.58	1.34	1.39
2	A	361	NBD	CB7-CB2	2.57	1.44	1.38
2	D	361	NBD	CB7-CB2	2.56	1.44	1.38
2	B	361	NBD	CB5-CB4	2.53	1.43	1.38
2	C	361	NBD	CB5-CB6	2.52	1.43	1.38
2	A	361	NBD	CB5-CB6	2.51	1.43	1.38
2	C	361	NBD	CB5-CB4	2.50	1.43	1.38
2	D	361	NBD	CB5-CB6	2.50	1.43	1.38
2	A	361	NBD	CB5-CB4	2.49	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	361	NBD	CB5-CB6	2.48	1.43	1.38
2	D	361	NBD	CB5-CB4	2.48	1.43	1.38
2	A	361	NBD	C6N-N1N	2.29	1.40	1.35
2	C	361	NBD	C6N-N1N	2.28	1.40	1.35
2	B	361	NBD	C6N-N1N	2.27	1.40	1.35
2	D	361	NBD	C6N-N1N	2.25	1.40	1.35
2	D	361	NBD	C3N-C7N	2.16	1.53	1.50
2	A	361	NBD	C3N-C7N	2.12	1.53	1.50
2	B	361	NBD	C3N-C7N	2.10	1.53	1.50
2	C	361	NBD	C3N-C7N	2.07	1.53	1.50

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	361	NBD	N3A-C2A-N1A	-7.11	117.81	128.58
2	A	361	NBD	N3A-C2A-N1A	-7.09	117.84	128.58
2	C	361	NBD	N3A-C2A-N1A	-7.07	117.87	128.58
2	D	361	NBD	N3A-C2A-N1A	-7.07	117.87	128.58
2	B	361	NBD	C2A-N3A-C4A	3.67	120.78	111.83
2	A	361	NBD	C2A-N3A-C4A	3.65	120.74	111.83
2	C	361	NBD	C2A-N3A-C4A	3.64	120.73	111.83
2	D	361	NBD	C2A-N3A-C4A	3.64	120.72	111.83
2	B	361	NBD	C5A-C4A-N3A	-3.56	121.82	126.72
2	C	361	NBD	C5A-C4A-N3A	-3.55	121.83	126.72
2	D	361	NBD	C5A-C4A-N3A	-3.54	121.84	126.72
2	A	361	NBD	C5A-C4A-N3A	-3.53	121.85	126.72
2	A	361	NBD	CB1-N6A-C6A	3.02	126.99	123.08
2	D	361	NBD	CB1-N6A-C6A	3.01	126.98	123.08
2	B	361	NBD	CB1-N6A-C6A	3.00	126.96	123.08
2	C	361	NBD	CB1-N6A-C6A	3.00	126.96	123.08
2	B	361	NBD	C2A-N1A-C6A	2.74	124.33	115.24
2	A	361	NBD	C2A-N1A-C6A	2.74	124.33	115.24
2	D	361	NBD	C2A-N1A-C6A	2.73	124.30	115.24
2	C	361	NBD	C2A-N1A-C6A	2.73	124.29	115.24
2	D	361	NBD	O12-PA-O3	2.51	114.06	107.27
2	B	361	NBD	C5A-C6A-N6A	2.51	126.88	122.03
2	C	361	NBD	O12-PA-O3	2.51	114.05	107.27
2	A	361	NBD	O12-PA-O3	2.51	114.05	107.27
2	C	361	NBD	C5A-C6A-N6A	2.50	126.86	122.03
2	B	361	NBD	O12-PA-O3	2.49	114.00	107.27
2	A	361	NBD	C5A-C6A-N6A	2.48	126.81	122.03
2	D	361	NBD	C5A-C6A-N6A	2.47	126.80	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	361	NBD	N9A-C8A-N7A	-2.21	110.80	113.94
2	A	361	NBD	N9A-C8A-N7A	-2.21	110.80	113.94
2	B	361	NBD	C2N-N1N-C1D	2.21	124.00	119.13
2	A	361	NBD	C2N-N1N-C1D	2.21	124.00	119.13
2	C	361	NBD	C2N-N1N-C1D	2.20	123.99	119.13
2	D	361	NBD	C2N-N1N-C1D	2.20	123.99	119.13
2	D	361	NBD	N3A-C4A-N9A	2.19	130.90	127.17
2	B	361	NBD	N3A-C4A-N9A	2.19	130.89	127.17
2	B	361	NBD	N9A-C8A-N7A	-2.18	110.84	113.94
2	A	361	NBD	N3A-C4A-N9A	2.17	130.87	127.17
2	C	361	NBD	N9A-C8A-N7A	-2.17	110.85	113.94
2	C	361	NBD	N3A-C4A-N9A	2.16	130.84	127.17
2	D	361	NBD	C2B-C1B-N9A	2.15	118.64	113.30
2	D	361	NBD	CB1-CB2-CB7	-2.13	116.58	120.94
2	C	361	NBD	C2B-C1B-N9A	2.13	118.61	113.30
2	A	361	NBD	C2B-C1B-N9A	2.13	118.60	113.30
2	B	361	NBD	C2B-C1B-N9A	2.13	118.59	113.30
2	A	361	NBD	CB1-CB2-CB7	-2.12	116.60	120.94
2	C	361	NBD	CB1-CB2-CB7	-2.12	116.61	120.94
2	B	361	NBD	CB1-CB2-CB7	-2.10	116.64	120.94
2	B	361	NBD	C6N-N1N-C2N	-2.09	120.10	121.88
2	D	361	NBD	C6N-N1N-C2N	-2.08	120.11	121.88
2	D	361	NBD	CB6-CB5-CB4	2.08	122.72	119.87
2	A	361	NBD	C6N-N1N-C2N	-2.08	120.11	121.88
2	B	361	NBD	CB6-CB5-CB4	2.07	122.71	119.87
2	D	361	NBD	CB7-CB2-CB3	2.07	121.31	118.23
2	C	361	NBD	C6N-N1N-C1D	-2.06	115.68	119.73
2	C	361	NBD	C6N-N1N-C2N	-2.06	120.13	121.88
2	A	361	NBD	C6N-N1N-C1D	-2.06	115.69	119.73
2	A	361	NBD	CB7-CB2-CB3	2.06	121.29	118.23
2	C	361	NBD	CB7-CB2-CB3	2.05	121.29	118.23
2	B	361	NBD	C6N-N1N-C1D	-2.05	115.70	119.73
2	A	361	NBD	CB6-CB5-CB4	2.05	122.68	119.87
2	D	361	NBD	C6N-N1N-C1D	-2.05	115.70	119.73
2	B	361	NBD	CB7-CB2-CB3	2.03	121.25	118.23
2	C	361	NBD	CB6-CB5-CB4	2.03	122.64	119.87

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	361	NBD	C5B-O5B-PA-O11

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Mol	Chain	Res	Type	Atoms
2	A	361	NBD	O4D-C1D-N1N-C2N
2	A	361	NBD	O4D-C1D-N1N-C6N
2	B	361	NBD	C5B-O5B-PA-O11
2	B	361	NBD	O4D-C1D-N1N-C2N
2	B	361	NBD	O4D-C1D-N1N-C6N
2	C	361	NBD	C5B-O5B-PA-O11
2	C	361	NBD	O4D-C1D-N1N-C2N
2	C	361	NBD	O4D-C1D-N1N-C6N
2	D	361	NBD	C5B-O5B-PA-O11
2	D	361	NBD	O4D-C1D-N1N-C2N
2	D	361	NBD	O4D-C1D-N1N-C6N
2	A	361	NBD	N1A-C6A-N6A-CB1
2	B	361	NBD	N1A-C6A-N6A-CB1
2	C	361	NBD	N1A-C6A-N6A-CB1
2	D	361	NBD	N1A-C6A-N6A-CB1
2	A	361	NBD	C5A-C6A-N6A-CB1
2	B	361	NBD	C5A-C6A-N6A-CB1
2	C	361	NBD	C5A-C6A-N6A-CB1
2	D	361	NBD	C5A-C6A-N6A-CB1
2	A	361	NBD	C2B-C1B-N9A-C8A
2	B	361	NBD	C2B-C1B-N9A-C8A
2	C	361	NBD	C2B-C1B-N9A-C8A
2	D	361	NBD	C2B-C1B-N9A-C8A
2	A	361	NBD	C2D-C1D-N1N-C2N
2	B	361	NBD	C2D-C1D-N1N-C2N
2	C	361	NBD	C2D-C1D-N1N-C2N
2	D	361	NBD	C2D-C1D-N1N-C2N
2	A	361	NBD	O4B-C1B-N9A-C8A
2	B	361	NBD	O4B-C1B-N9A-C8A
2	C	361	NBD	O4B-C1B-N9A-C8A
2	D	361	NBD	O4B-C1B-N9A-C8A
2	A	361	NBD	C2B-C1B-N9A-C4A
2	B	361	NBD	C2B-C1B-N9A-C4A
2	C	361	NBD	C2B-C1B-N9A-C4A
2	D	361	NBD	C2B-C1B-N9A-C4A
2	A	361	NBD	PA-O3-PN-O13
2	B	361	NBD	PA-O3-PN-O13
2	C	361	NBD	PA-O3-PN-O13
2	D	361	NBD	PA-O3-PN-O13
2	A	361	NBD	O4B-C4B-C5B-O5B
2	B	361	NBD	O4B-C4B-C5B-O5B
2	C	361	NBD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	361	NBD	O4B-C4B-C5B-O5B

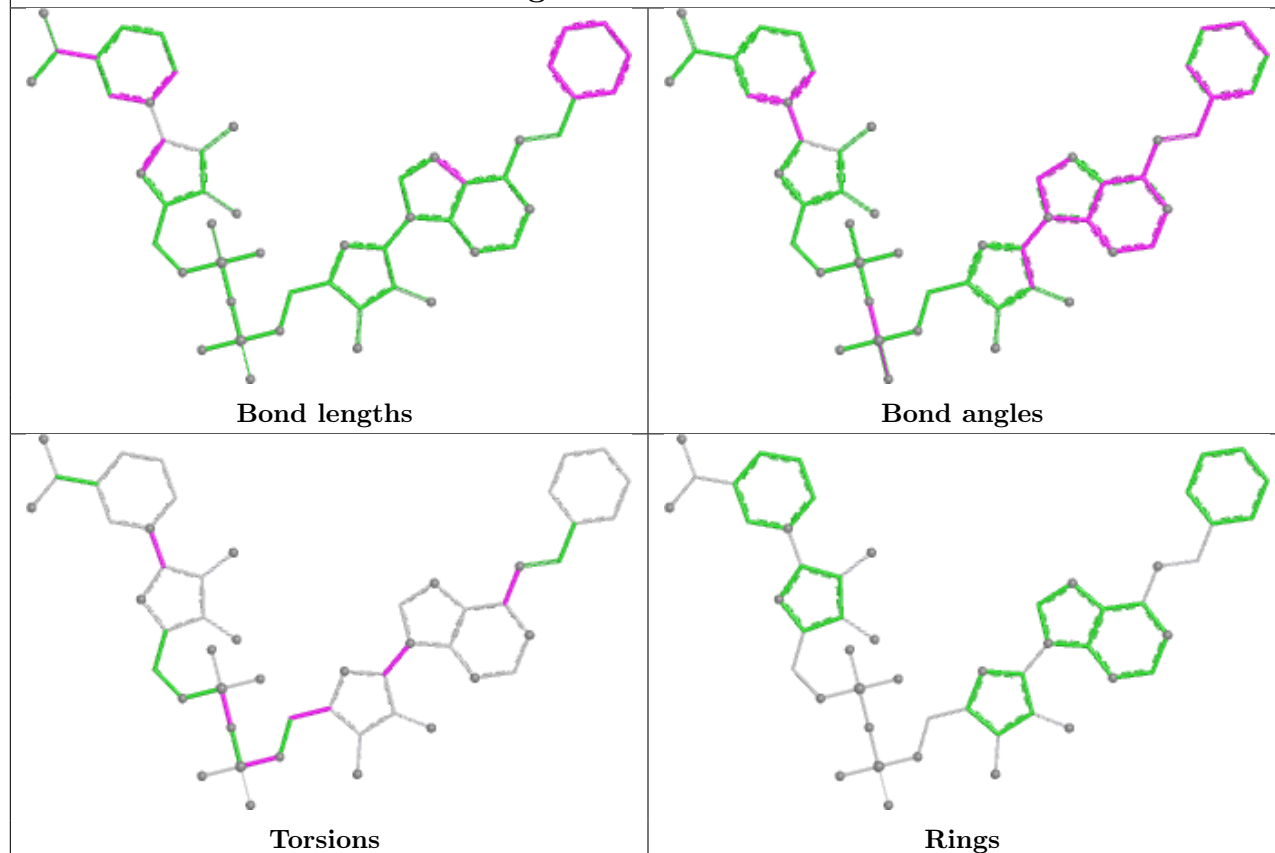
There are no ring outliers.

4 monomers are involved in 31 short contacts:

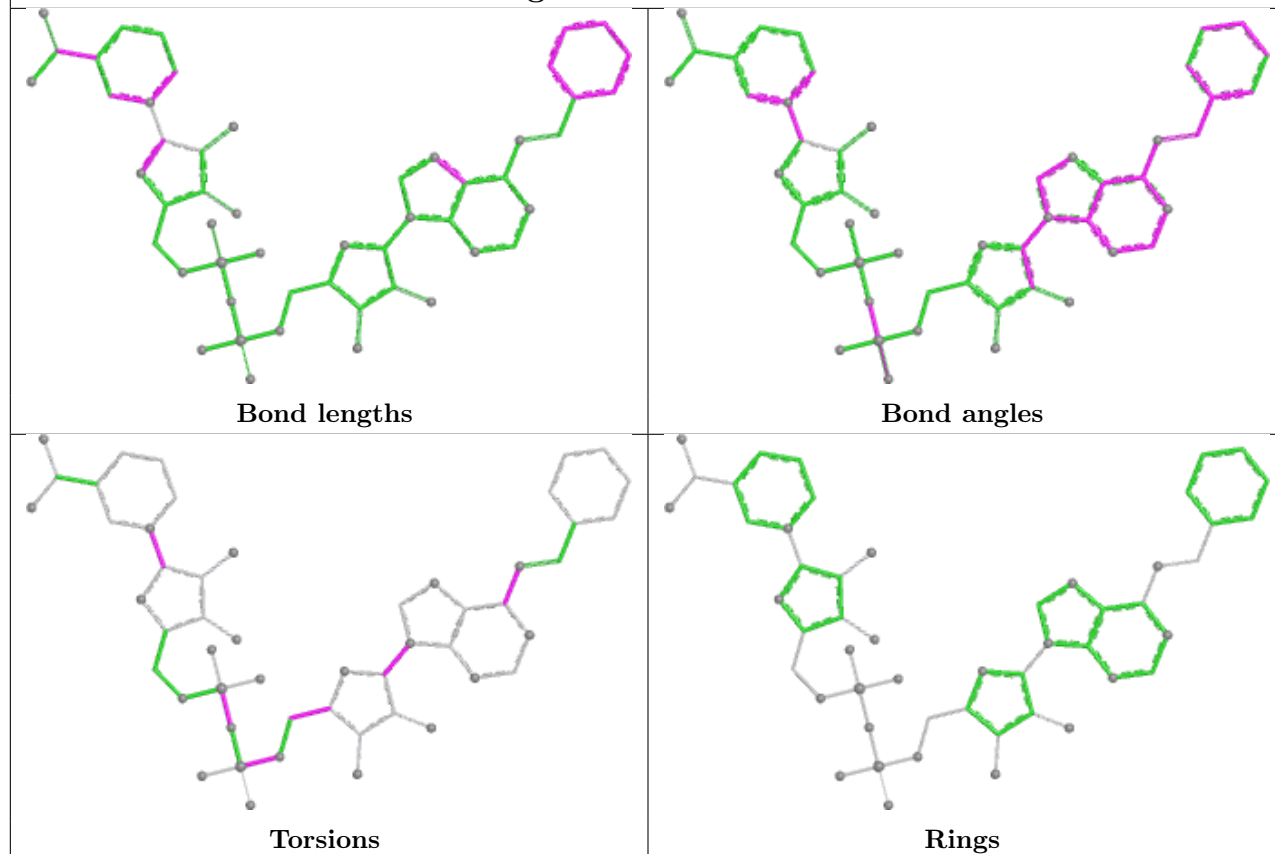
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	361	NBD	7	0
2	D	361	NBD	9	0
2	B	361	NBD	5	0
2	A	361	NBD	10	0

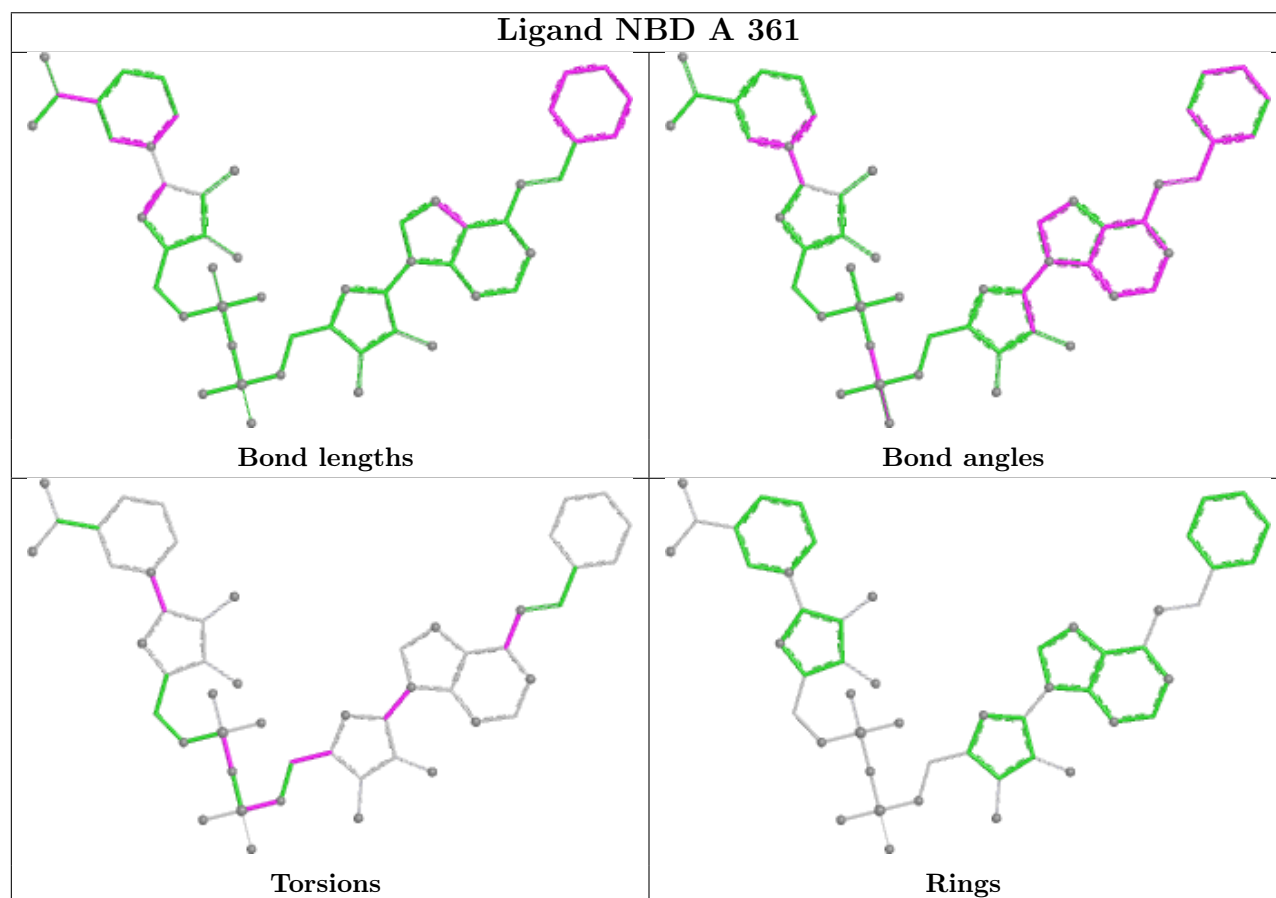
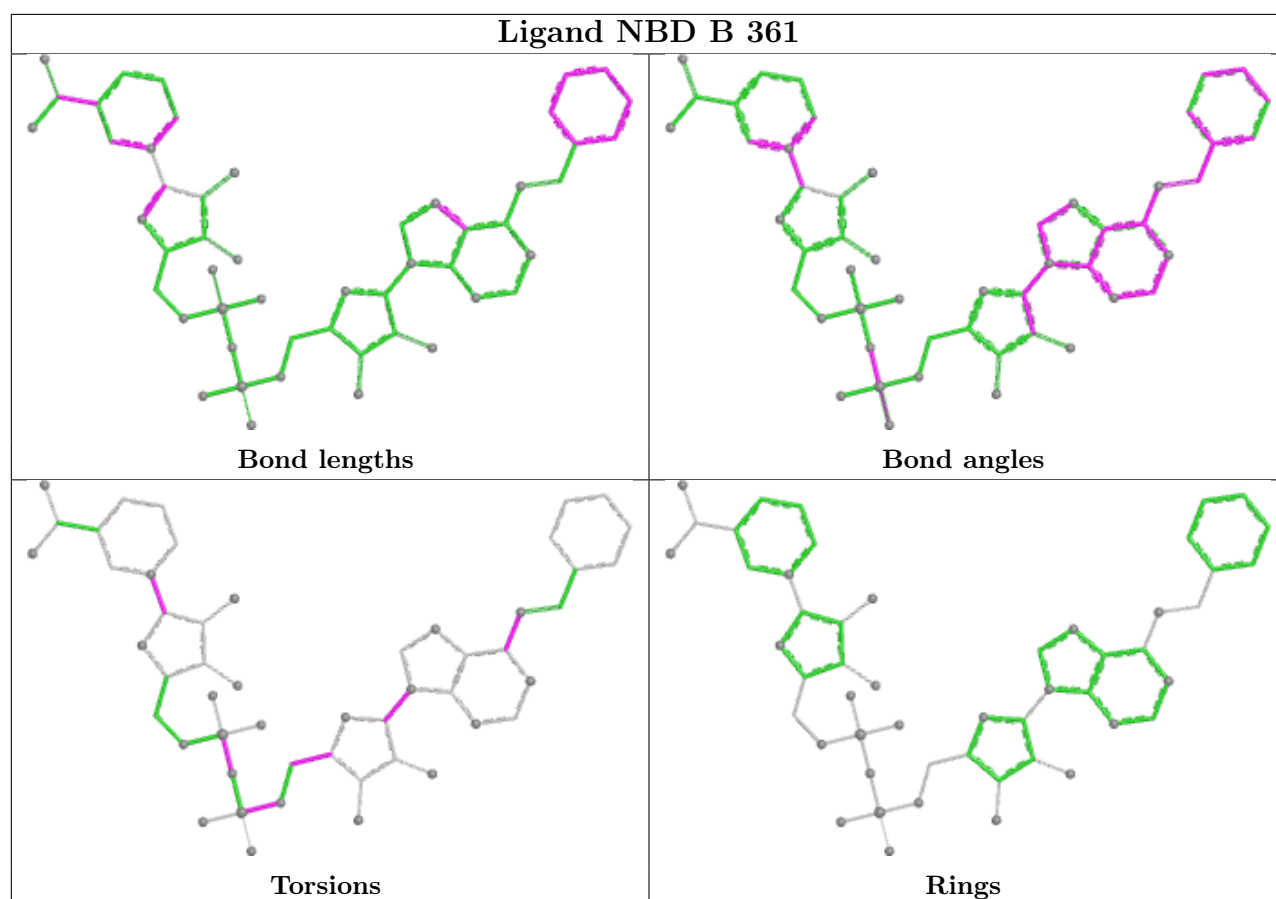
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand NBD C 361



Ligand NBD D 361





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.