



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:43 PM GMT

PDB ID : 1GYQ  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

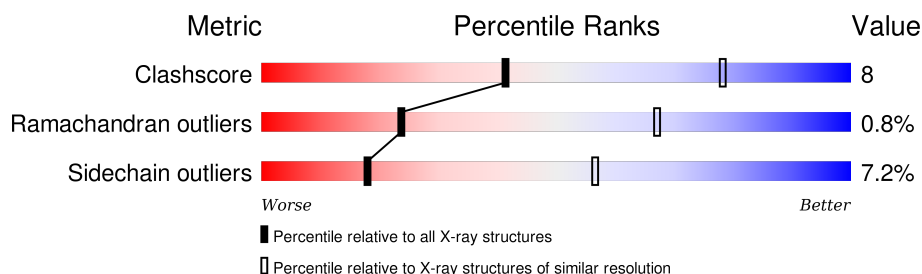
# 1 Overall quality at a glance

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	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	358	 69% 27% .
1	B	358	 79% 19% .
1	C	358	 72% 25% . .
1	D	358	 74% 23% .

## 2 Entry composition [i](#)

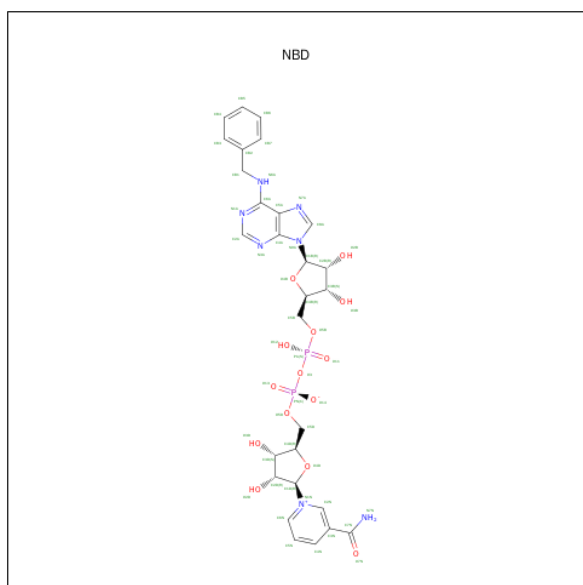
There are 2 unique types of molecules in this entry. The entry contains 11068 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: NBD) (formula: C<sub>28</sub>H<sub>33</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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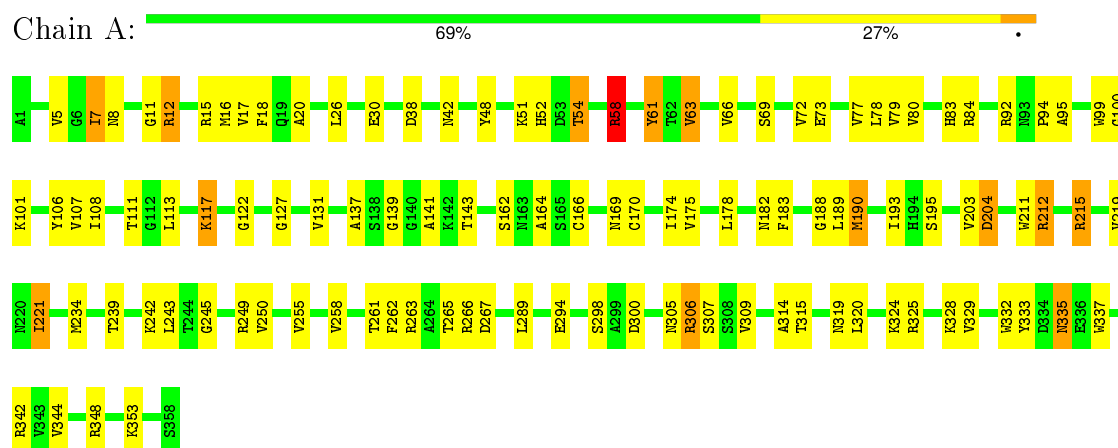
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			51	28	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			51	28	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			51	28	7	14	2		

### 3 Residue-property plots

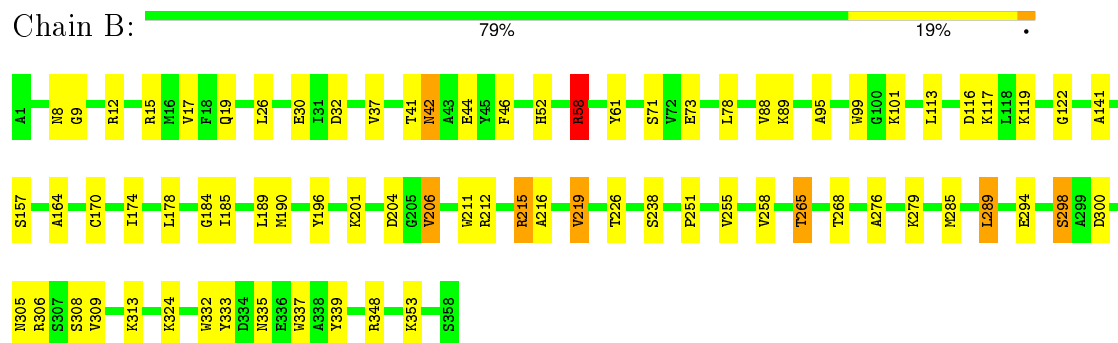
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

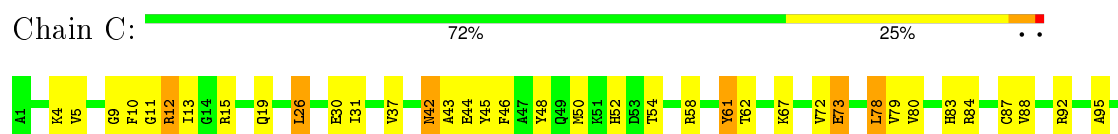
- Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

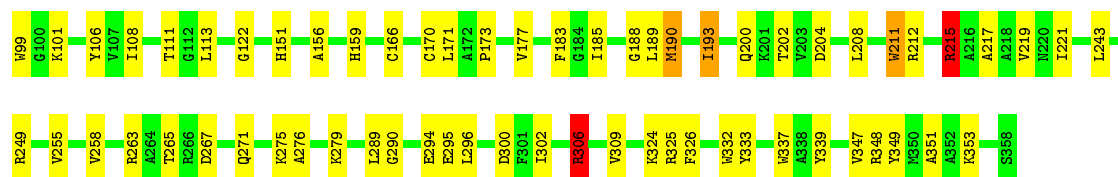


- Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)



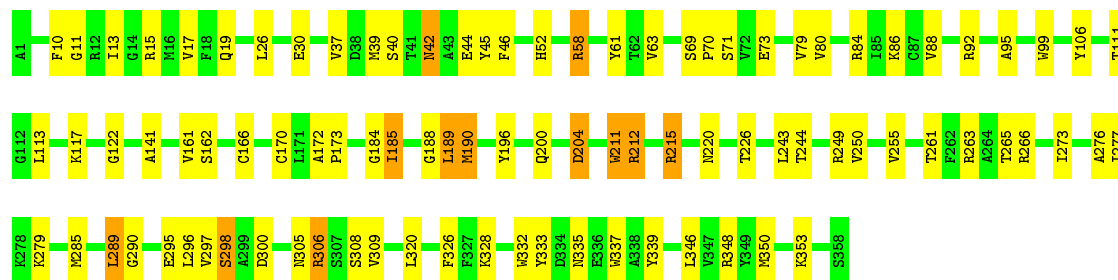
- Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)





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

Chain D: 74% 23% .



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	0.75	0/2768	1.48	34/3752 (0.9%)
1	B	0.79	0/2768	1.44	26/3752 (0.7%)
1	C	0.75	0/2768	1.47	33/3752 (0.9%)
1	D	0.77	0/2768	1.43	24/3752 (0.6%)
All	All	0.76	0/11072	1.45	117/15008 (0.8%)

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

There are no bond length outliers.

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	ARG	NE-CZ-NH1	13.33	126.97	120.30
1	A	215	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	C	215	ARG	NE-CZ-NH2	-9.91	115.35	120.30
1	C	332	TRP	CD1-CG-CD2	9.63	114.00	106.30
1	D	332	TRP	CD1-CG-CD2	9.42	113.84	106.30
1	B	332	TRP	CD1-CG-CD2	9.39	113.82	106.30
1	B	99	TRP	CD1-CG-CD2	8.92	113.43	106.30
1	D	99	TRP	CD1-CG-CD2	8.88	113.40	106.30
1	A	337	TRP	CD1-CG-CD2	8.84	113.37	106.30
1	D	215	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	D	337	TRP	CD1-CG-CD2	8.50	113.10	106.30
1	A	332	TRP	CD1-CG-CD2	8.47	113.07	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	TRP	CE2-CD2-CG	-8.31	100.65	107.30
1	A	99	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	C	332	TRP	CE2-CD2-CG	-8.10	100.82	107.30
1	B	99	TRP	CE2-CD2-CG	-8.07	100.84	107.30
1	A	99	TRP	CE2-CD2-CG	-7.98	100.92	107.30
1	B	337	TRP	CD1-CG-CD2	7.98	112.68	106.30
1	A	332	TRP	CE2-CD2-CG	-7.92	100.96	107.30
1	D	99	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	C	99	TRP	CD1-CG-CD2	7.84	112.58	106.30
1	C	337	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	C	15	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	337	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	C	99	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	D	337	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	C	211	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	B	348	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	D	332	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	C	337	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	D	215	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	D	211	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	B	337	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	A	99	TRP	CG-CD2-CE3	7.17	140.35	133.90
1	D	348	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	D	211	TRP	CD1-CG-CD2	7.12	111.99	106.30
1	C	99	TRP	CG-CD2-CE3	7.03	140.23	133.90
1	B	15	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	B	211	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	C	211	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	B	332	TRP	CG-CD2-CE3	6.88	140.09	133.90
1	A	58	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	C	306	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	D	15	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	211	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	A	12	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	D	15	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	C	249	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	C	249	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	332	TRP	CG-CD1-NE1	-6.40	103.70	110.10
1	B	211	TRP	CD1-CG-CD2	6.40	111.42	106.30
1	A	325	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	99	TRP	CB-CG-CD1	-6.29	118.82	127.00
1	B	332	TRP	CB-CG-CD1	-6.28	118.83	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	D	332	TRP	CG-CD1-NE1	-6.21	103.89	110.10
1	B	332	TRP	CG-CD1-NE1	-6.19	103.91	110.10
1	D	339	TYR	CB-CG-CD1	-6.19	117.29	121.00
1	D	266	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	263	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	99	TRP	CB-CG-CD1	-6.08	119.10	127.00
1	D	348	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	266	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	D	99	TRP	CG-CD2-CE3	6.04	139.34	133.90
1	A	16	MET	CG-SD-CE	6.02	109.83	100.20
1	A	211	TRP	CD1-CG-CD2	5.96	111.07	106.30
1	C	348	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	15	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	B	206	VAL	CG1-CB-CG2	-5.85	101.54	110.90
1	A	58	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	D	92	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	211	TRP	CG-CD2-CE3	5.78	139.10	133.90
1	A	215	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	234	MET	CA-CB-CG	5.75	123.07	113.30
1	D	266	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	212	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	348	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	58	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	212	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	166	CYS	CA-CB-SG	5.68	124.23	114.00
1	B	58	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	219	VAL	N-CA-CB	-5.64	99.08	111.50
1	A	221	ILE	N-CA-C	-5.61	95.86	111.00
1	D	211	TRP	CG-CD2-CE3	5.58	138.93	133.90
1	A	249	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	99	TRP	CG-CD2-CE3	5.52	138.86	133.90
1	A	92	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	99	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	C	325	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	306	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	339	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	A	99	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	A	203	VAL	CG1-CB-CG2	-5.43	102.20	110.90
1	A	193	ILE	N-CA-C	-5.42	96.38	111.00
1	C	92	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	306	ARG	NE-CZ-NH2	-5.36	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	TYR	CB-CG-CD2	-5.34	117.79	121.00
1	B	215	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	D	99	TRP	CB-CG-CD1	-5.33	120.08	127.00
1	C	99	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	B	17	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	C	48	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	212	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	332	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	B	196	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	C	193	ILE	N-CA-C	-5.24	96.84	111.00
1	B	32	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	182	ASN	N-CA-C	5.21	125.07	111.00
1	C	84	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	51	LYS	CB-CG-CD	-5.15	98.22	111.60
1	C	302	ILE	CA-C-N	-5.14	105.89	117.20
1	C	12	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	313	LYS	CA-CB-CG	-5.12	102.13	113.40
1	B	15	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	339	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	A	61	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	C	61	TYR	CB-CG-CD2	-5.07	117.96	121.00

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	68	0
1	B	2716	0	2736	44	0
1	C	2716	0	2736	59	0
1	D	2716	0	2736	60	0
2	A	51	0	32	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	51	0	32	4	0
2	C	51	0	32	6	0
2	D	51	0	32	9	0
All	All	11068	0	11072	188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (188) 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:C:113:LEU:HD12	2:C:361:NBD:HB11	1.65	0.77
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:VAL:HG22	1:C:88:VAL:HB	1.88	0.56
1:A:267:ASP:HB3	1:A:324:LYS:HD2	1.87	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
1:A:320:LEU:HG	1:D:244:THR:HG22	1.88	0.55
1:A:66:VAL:HG23	1:A:77:VAL:HB	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:C:113:LEU:CD1	2:C:361:NBD:HB11	2.38	0.52
1:C:9:GLY:HA2	2:C:361:NBD:N3A	2.25	0.52
1:A:258:VAL:HG23	1:A:333:TYR:HE1	1.75	0.52
1:A:242:LYS:O	1:D:320:LEU:HD11	2.10	0.52
1:A:188:GLY:HA2	1:D:326:PHE:CE1	2.45	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:B:258:VAL:HG23	1:B:333:TYR:CE1	2.45	0.51
1:A:69:SER:O	1:A:72:VAL:HG22	2.10	0.51
1:B:204:ASP:OD2	1:B:215:ARG:HD2	2.11	0.51
1:A:250:VAL:HG11	1:D:250:VAL:HG11	1.91	0.51
1:A:117:LYS:HG2	1:A:139:GLY:O	2.10	0.51
1:A:18:PHE:CZ	1:A:80:VAL:HG21	2.46	0.50
1:A:262:PHE:HE1	1:A:329:VAL:HG23	1.77	0.50
1:A:52:HIS:HE1	1:C:294:GLU:OE1	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:THR:CG2	2:D:361:NBD:C2A	2.91	0.49
1:D:190:MET:HE2	1:D:226:THR:HG21	1.93	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
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:B:190:MET:HE3	1:B:226:THR:HG21	1.96	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: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:C:26:LEU:HB3	1:C:31:ILE:HB	1.96	0.47
1:A:79:VAL:HG22	1:A:84:ARG:HG2	1.97	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:113:LEU:HD12	2:B:361:NBD:HB11	1.97	0.46
1:B:19:GLN:HG3	1:B:61:TYR:CE2	2.50	0.46
1:B:117:LYS:HB2	1:B:141:ALA:HB2	1.97	0.46
1:C:78:LEU:HD22	1:C:87:CYS:SG	2.55	0.46
1:A:52:HIS:HD2	1:A:58:ARG:NH1	2.13	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:D:290:GLY:HA3	1:D:306:ARG:NH1	2.32	0.45
1:B:285:MET:HB3	1:B:289:LEU:HB2	1.98	0.45
1:B:42:ASN:ND2	1:B:44:GLU:HB2	2.32	0.45
1:C:170:CYS:SG	1:C:333:TYR:CD1	3.09	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:HIS:CE1	1:C:296:LEU:HD21	2.51	0.45
1:D:39:MET:CE	2:D:361:NBD:CB5	2.95	0.45
1:C:188:GLY:O	1:C:243:LEU:HA	2.17	0.45
1:B:9:GLY:HA2	2:B:361:NBD:N3A	2.32	0.45
1:A:52:HIS:HD2	1:A:58:ARG:HH11	1.65	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
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:D:19:GLN:HG3	1:D:61:TYR:HE2	1.83	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:N	1:C:193:ILE:HD12	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:39:MET:HE1	2:D:361:NBD:CB5	2.49	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:B:300:ASP:OD1	1:C:215:ARG:NH2	2.48	0.43
1:A:170:CYS:SG	1:A:333:TYR:CD1	3.12	0.43
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:C:276:ALA:HA	1:C:279:LYS:HE2	2.01	0.42
1:C:200:GLN:HB3	1:C:217:ALA:HB2	2.00	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:C:73:GLU:H	1:C:73:GLU:CD	2.23	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:C:5:VAL:HA	1:C:106:TYR:O	2.19	0.42
1:B:174:ILE:O	1:B:178:LEU:HG	2.20	0.42
1:B:215:ARG:NH2	1:C:300:ASP:OD2	2.52	0.41
1:C:54:THR:HB	1:D:204:ASP:OD1	2.20	0.41
1:B:294:GLU:OE2	1:D:52:HIS:HE1	2.03	0.41
1:D:285:MET:HB3	1:D:289:LEU:HB2	2.02	0.41
1:A:48:TYR:CE1	1:C:295:GLU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:CD1	2:B:361:NBD:HB11	2.50	0.41
1:A:54:THR:HB	1:B:204:ASP:OD1	2.20	0.41
1:B:37:VAL:HG22	1:B:88:VAL:HB	2.02	0.41
1:D:95:ALA:HA	1:D:122:GLY:O	2.20	0.41
1:B:42:ASN:ND2	1:B:44:GLU:H	2.18	0.41
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: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:D:63:VAL:HG13	1:D:80:VAL:HG22	2.02	0.41
1:A:100:GLY:H	1:A:127:GLY:HA3	1.85	0.41
1:D:161:VAL:HG21	1:D:350:MET:SD	2.61	0.41
1:D:11:GLY:HA3	2:D:361:NBD:O5B	2.21	0.41
1:C:106:TYR:OH	1:C:351:ALA:HA	2.20	0.41
1:C:46:PHE:O	1:C:50:MET:SD	2.79	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:12:ARG:NH1	1:D:204:ASP:HB2	2.36	0.41
1:D:106:TYR:N	1:D:106:TYR:CD1	2.89	0.41
1:C:67:LYS:HB3	1:C:72:VAL:CG2	2.51	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:D:185:ILE:HD11	1:D:243:LEU:HB2	2.02	0.40
1:B:189:LEU:HB2	1:C:326:PHE:CE1	2.56	0.40
1:A:204:ASP:HB2	1:B:12:ARG:HH11	1.87	0.40
1:D:42:ASN:ND2	1:D:44:GLU:H	2.19	0.40
1:B:201:LYS:HE3	1:B:206:VAL:O	2.22	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:B:52:HIS:HD2	1:B:58:ARG:NH1	2.19	0.40
1:D:170:CYS:SG	1:D:333:TYR:CD1	3.15	0.40
1:C:42:ASN:ND2	1:C:44:GLU:HB2	2.37	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	356/358 (99%)	325 (91%)	27 (8%)	4 (1%)	17	61
1	B	356/358 (99%)	333 (94%)	20 (6%)	3 (1%)	24	67
1	C	356/358 (99%)	330 (93%)	25 (7%)	1 (0%)	46	82
1	D	356/358 (99%)	332 (93%)	21 (6%)	3 (1%)	24	67
All	All	1424/1432 (99%)	1320 (93%)	93 (6%)	11 (1%)	24	67

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

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%)	271 (92%)	23 (8%)	16	52
1	B	294/294 (100%)	275 (94%)	19 (6%)	21	61
1	C	294/294 (100%)	274 (93%)	20 (7%)	20	60
1	D	294/294 (100%)	271 (92%)	23 (8%)	16	52
All	All	1176/1176 (100%)	1091 (93%)	85 (7%)	18	56

All (85) 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	38	ASP
1	A	42	ASN
1	A	54	THR
1	A	58	ARG
1	A	63	VAL
1	A	73	GLU
1	A	78	LEU
1	A	94	PRO
1	A	101	LYS
1	A	190	MET
1	A	195	SER
1	A	204	ASP
1	A	289	LEU
1	A	305	ASN
1	A	306	ARG
1	A	309	VAL
1	A	319	ASN
1	A	335	ASN
1	A	348	ARG
1	A	353	LYS
1	B	26	LEU
1	B	30	GLU
1	B	42	ASN
1	B	58	ARG
1	B	71	SER
1	B	73	GLU
1	B	78	LEU
1	B	101	LYS
1	B	157	SER
1	B	185	ILE

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Mol	Chain	Res	Type
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	306	ARG
1	B	309	VAL
1	B	353	LYS
1	C	4	LYS
1	C	26	LEU
1	C	30	GLU
1	C	42	ASN
1	C	58	ARG
1	C	73	GLU
1	C	78	LEU
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	289	LEU
1	C	306	ARG
1	C	309	VAL
1	C	353	LYS
1	D	26	LEU
1	D	30	GLU
1	D	42	ASN
1	D	58	ARG
1	D	69	SER
1	D	71	SER
1	D	73	GLU
1	D	86	LYS
1	D	162	SER
1	D	166	CYS
1	D	185	ILE
1	D	189	LEU
1	D	190	MET

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Mol	Chain	Res	Type
1	D	204	ASP
1	D	212	ARG
1	D	265	THR
1	D	289	LEU
1	D	298	SER
1	D	305	ASN
1	D	306	ARG
1	D	309	VAL
1	D	335	ASN
1	D	353	LYS

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	42	ASN
1	A	52	HIS
1	A	159	HIS
1	A	305	ASN
1	B	8	ASN
1	B	42	ASN
1	B	52	HIS
1	B	151	HIS
1	B	305	ASN
1	C	8	ASN
1	C	42	ASN
1	C	52	HIS
1	C	81	ASN
1	C	159	HIS
1	D	8	ASN
1	D	42	ASN
1	D	52	HIS
1	D	81	ASN
1	D	305	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	361	-	45,56,56	1.30	11 (24%)	58,83,83	2.79	8 (13%)
2	NBD	B	361	-	45,56,56	1.30	11 (24%)	58,83,83	2.80	8 (13%)
2	NBD	C	361	-	45,56,56	1.31	11 (24%)	58,83,83	2.79	8 (13%)
2	NBD	D	361	-	45,56,56	1.30	11 (24%)	58,83,83	2.79	8 (13%)

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	A	361	-	-	0/27/67/67	0/6/6/6
2	NBD	B	361	-	-	0/27/67/67	0/6/6/6
2	NBD	C	361	-	-	0/27/67/67	0/6/6/6
2	NBD	D	361	-	-	0/27/67/67	0/6/6/6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	361	NBD	C3N-C7N	2.00	1.53	1.50
2	B	361	NBD	C3N-C7N	2.03	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	361	NBD	C3N-C7N	2.05	1.53	1.50
2	D	361	NBD	O4B-C1B	2.07	1.43	1.41
2	D	361	NBD	C3N-C7N	2.08	1.53	1.50
2	A	361	NBD	O4B-C1B	2.09	1.43	1.41
2	B	361	NBD	O4B-C1B	2.09	1.43	1.41
2	C	361	NBD	O4B-C1B	2.11	1.43	1.41
2	D	361	NBD	C6A-N1A	2.16	1.37	1.34
2	C	361	NBD	CB4-CB3	2.16	1.43	1.38
2	B	361	NBD	CB4-CB3	2.16	1.43	1.38
2	A	361	NBD	CB6-CB7	2.17	1.43	1.38
2	B	361	NBD	CB6-CB7	2.17	1.43	1.38
2	A	361	NBD	CB4-CB3	2.17	1.43	1.38
2	C	361	NBD	CB6-CB7	2.18	1.43	1.38
2	D	361	NBD	CB6-CB7	2.18	1.43	1.38
2	A	361	NBD	C6A-N1A	2.19	1.37	1.34
2	D	361	NBD	CB4-CB3	2.19	1.43	1.38
2	D	361	NBD	CB5-CB4	2.21	1.43	1.38
2	B	361	NBD	CB5-CB6	2.21	1.43	1.38
2	A	361	NBD	CB5-CB4	2.22	1.43	1.38
2	C	361	NBD	C6A-N1A	2.22	1.37	1.34
2	B	361	NBD	C6A-N1A	2.22	1.37	1.34
2	D	361	NBD	CB5-CB6	2.22	1.43	1.38
2	C	361	NBD	CB5-CB4	2.23	1.43	1.38
2	A	361	NBD	CB5-CB6	2.23	1.43	1.38
2	C	361	NBD	CB5-CB6	2.24	1.43	1.38
2	B	361	NBD	CB5-CB4	2.25	1.43	1.38
2	D	361	NBD	CB7-CB2	2.43	1.44	1.38
2	A	361	NBD	CB7-CB2	2.44	1.44	1.38
2	B	361	NBD	CB7-CB2	2.44	1.44	1.38
2	C	361	NBD	CB7-CB2	2.45	1.44	1.38
2	B	361	NBD	O4D-C1D	2.57	1.44	1.41
2	C	361	NBD	C2A-N3A	2.57	1.36	1.32
2	D	361	NBD	O4D-C1D	2.58	1.44	1.41
2	A	361	NBD	O4D-C1D	2.59	1.44	1.41
2	B	361	NBD	C2A-N3A	2.59	1.36	1.32
2	A	361	NBD	C2A-N3A	2.61	1.36	1.32
2	C	361	NBD	O4D-C1D	2.61	1.44	1.41
2	D	361	NBD	C2A-N3A	2.61	1.36	1.32
2	A	361	NBD	CB3-CB2	2.63	1.44	1.38
2	D	361	NBD	CB3-CB2	2.63	1.44	1.38
2	B	361	NBD	CB3-CB2	2.64	1.44	1.38
2	C	361	NBD	CB3-CB2	2.65	1.44	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	361	NBD	N3A-C2A-N1A	-14.47	117.81	128.89
2	A	361	NBD	N3A-C2A-N1A	-14.43	117.84	128.89
2	C	361	NBD	N3A-C2A-N1A	-14.39	117.87	128.89
2	D	361	NBD	N3A-C2A-N1A	-14.39	117.87	128.89
2	B	361	NBD	C4B-O4B-C1B	-2.88	106.55	109.72
2	C	361	NBD	C4B-O4B-C1B	-2.88	106.55	109.72
2	D	361	NBD	C4B-O4B-C1B	-2.86	106.58	109.72
2	A	361	NBD	C4B-O4B-C1B	-2.85	106.59	109.72
2	C	361	NBD	N6A-C6A-N1A	-2.48	115.71	119.14
2	B	361	NBD	N6A-C6A-N1A	-2.47	115.72	119.14
2	D	361	NBD	N6A-C6A-N1A	-2.46	115.73	119.14
2	A	361	NBD	N6A-C6A-N1A	-2.45	115.75	119.14
2	B	361	NBD	C2B-C1B-N9A	2.81	118.59	114.29
2	A	361	NBD	C2B-C1B-N9A	2.82	118.60	114.29
2	C	361	NBD	C2B-C1B-N9A	2.82	118.61	114.29
2	D	361	NBD	C2B-C1B-N9A	2.85	118.64	114.29
2	C	361	NBD	CB1-N6A-C6A	3.03	126.96	123.16
2	B	361	NBD	CB1-N6A-C6A	3.03	126.96	123.16
2	D	361	NBD	CB1-N6A-C6A	3.05	126.98	123.16
2	A	361	NBD	CB1-N6A-C6A	3.06	126.99	123.16
2	D	361	NBD	C5A-C6A-N6A	3.85	126.80	120.47
2	A	361	NBD	C5A-C6A-N6A	3.86	126.81	120.47
2	C	361	NBD	C5A-C6A-N6A	3.89	126.86	120.47
2	B	361	NBD	C5A-C6A-N6A	3.89	126.88	120.47
2	D	361	NBD	O4D-C1D-N1N	5.75	114.45	108.13
2	C	361	NBD	O4D-C1D-N1N	5.76	114.46	108.13
2	A	361	NBD	O4D-C1D-N1N	5.78	114.48	108.13
2	B	361	NBD	O4D-C1D-N1N	5.80	114.50	108.13
2	C	361	NBD	C2A-N1A-C6A	10.84	124.29	116.48
2	D	361	NBD	C2A-N1A-C6A	10.85	124.30	116.48
2	A	361	NBD	C2A-N1A-C6A	10.89	124.33	116.48
2	B	361	NBD	C2A-N1A-C6A	10.90	124.33	116.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	361	NBD	8	0

*Continued on next page...*

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	361	NBD	4	0
2	C	361	NBD	6	0
2	D	361	NBD	9	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.