



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:21 AM UTC

PDB ID : 3IDS / pdb_00003ids
Title : Structure of Glycosomal Glyceraldehyde-3-Phosphate Dehydrogenase from Trypanosoma cruzi in complex with the irreversible iodoacetamide inhibitor
Authors : Balliano, T.L.; Guido, R.V.C.; Andricopulo, A.D.; Oliva, G.
Deposited on : 2009-07-21
Resolution : 1.80 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

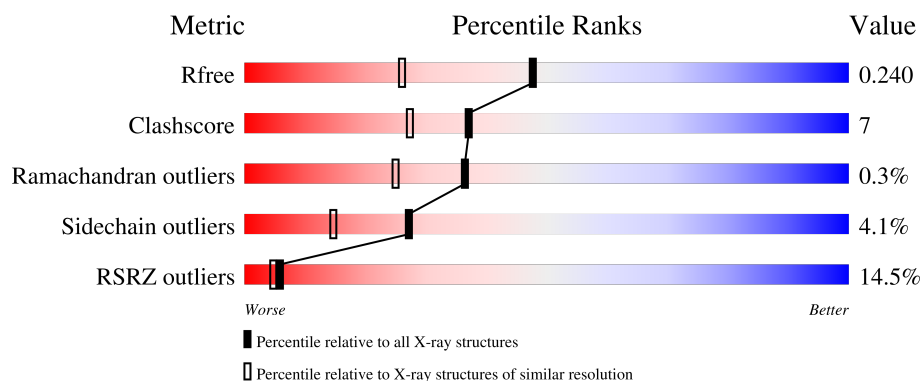
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	359	2% 81% 17% .
1	B	359	19% 85% 12% .
1	C	359	34% 83% 14% .
1	D	359	3% 85% 13% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACM	A	360	-	-	X	-
2	ACM	B	360	-	-	X	-
2	ACM	C	360	-	-	X	-

2 Entry composition [i](#)

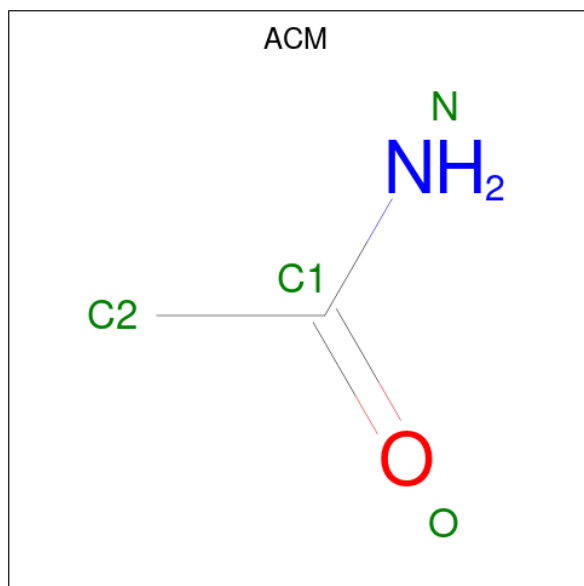
There are 5 unique types of molecules in this entry. The entry contains 12142 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, glycosomal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	359	Total	C	N	O	S	0	0	0
			2733	1717	483	520	13			
1	D	359	Total	C	N	O	S	1	0	0
			2733	1717	483	520	13			
1	A	359	Total	C	N	O	S	1	0	0
			2733	1717	483	520	13			
1	B	359	Total	C	N	O	S	0	0	0
			2733	1717	483	520	13			

- Molecule 2 is ACETAMIDE (CCD ID: ACM) (formula: C₂H₅NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			4	2	1	1		
2	A	1	Total	C	N	O	0	0
			4	2	1	1		

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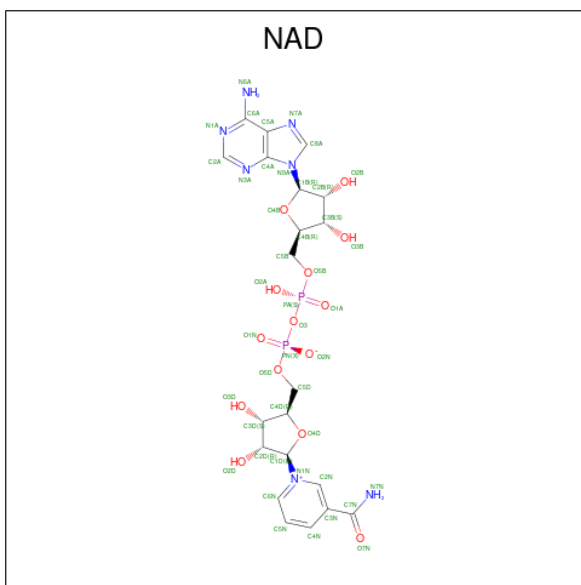
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

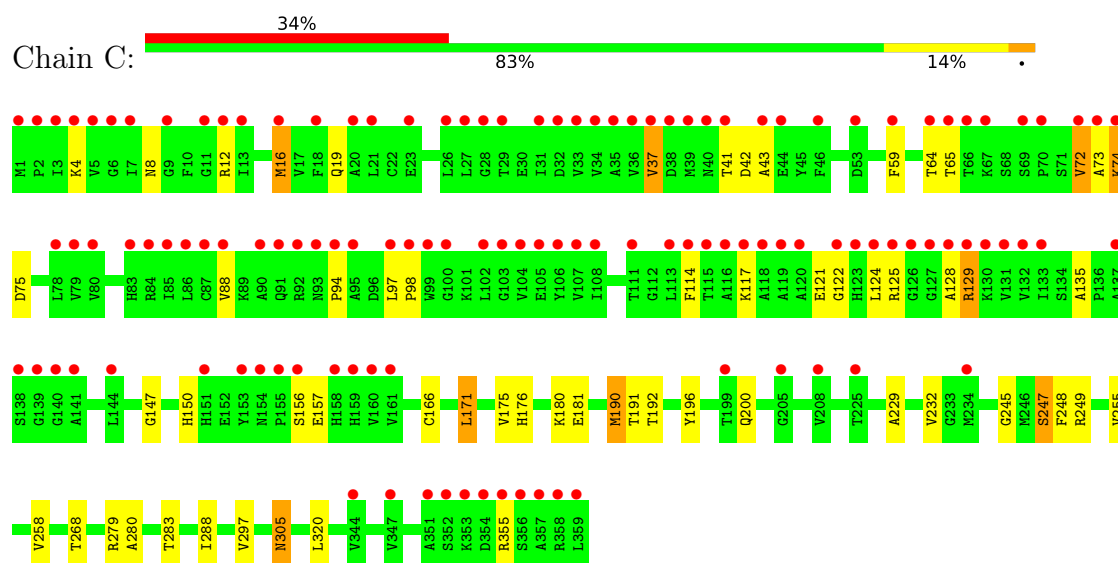
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	170	Total O 170 170	0	0
5	D	343	Total O 343 343	0	0
5	A	355	Total O 355 355	0	0
5	B	250	Total O 250 250	0	0

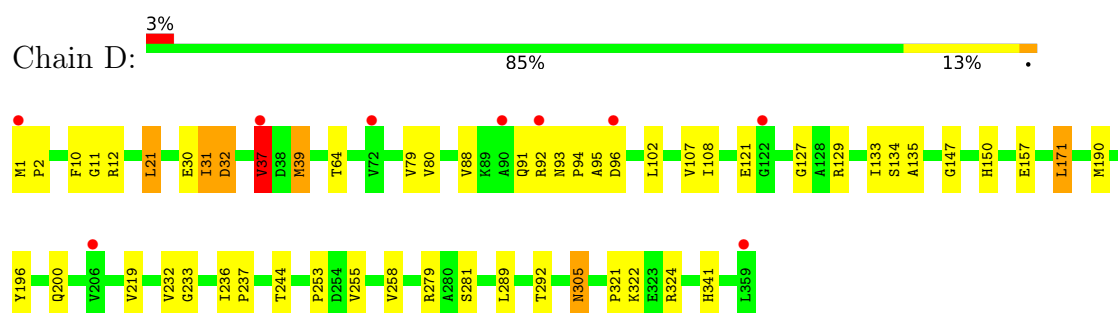
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

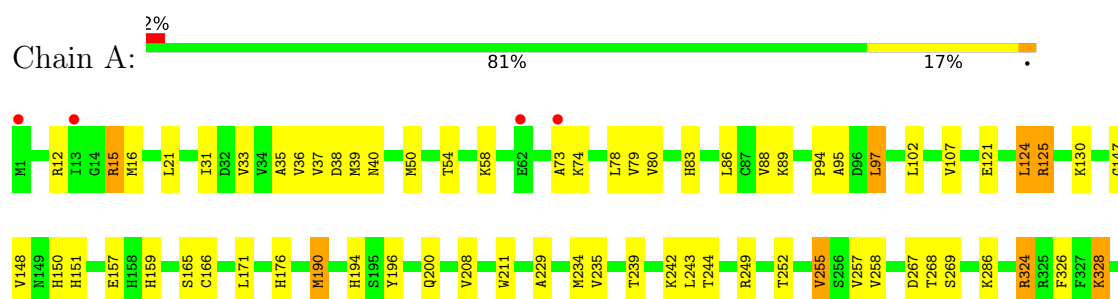
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal

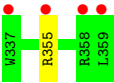


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal

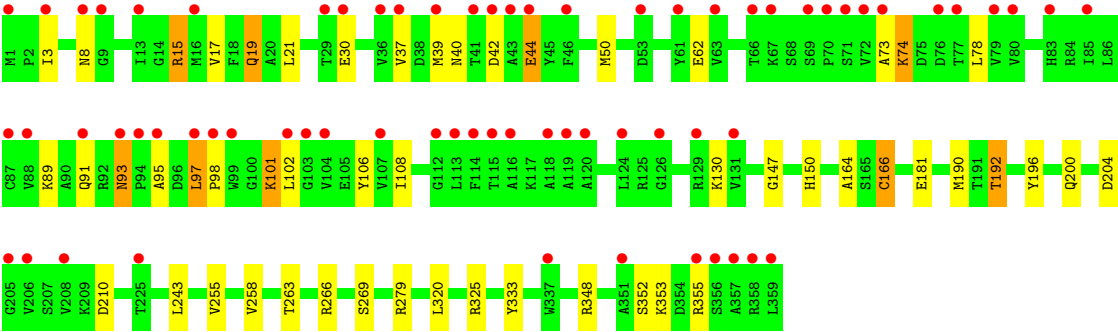
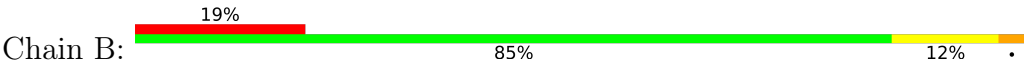


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal





● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.12Å 85.39Å 105.66Å 90.00° 96.42° 90.00°	Depositor
Resolution (Å)	61.66 – 1.80 61.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (61.66-1.80) 97.0 (61.66-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.200 , 0.240 (Not available) , 0.240	Depositor DCC
R_{free} test set	6629 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12142	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: ACM, GOL, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	23/2786 (0.8%)	0.85	0/3778
1	B	0.86	8/2786 (0.3%)	0.85	1/3778 (0.0%)
1	C	0.94	9/2786 (0.3%)	0.87	3/3778 (0.1%)
1	D	0.96	16/2786 (0.6%)	0.86	2/3778 (0.1%)
All	All	0.96	56/11144 (0.5%)	0.86	6/15112 (0.0%)

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	VAL	C-O	-7.92	1.15	1.24
1	A	257	VAL	C-O	-7.48	1.16	1.24
1	D	31	ILE	C-O	-6.95	1.16	1.24
1	C	268	THR	C-O	-6.94	1.17	1.24
1	B	164	ALA	C-O	-6.90	1.17	1.24
1	A	235	VAL	C-O	-6.68	1.17	1.24
1	A	267	ASP	C-O	-6.61	1.16	1.23
1	D	32	ASP	C-O	-6.55	1.16	1.24
1	B	21	LEU	C-O	-6.46	1.16	1.24
1	C	297	VAL	C-O	-6.21	1.16	1.23
1	A	73	ALA	CA-CB	-6.15	1.43	1.53
1	B	266	ARG	C-O	-6.15	1.16	1.23
1	D	133	ILE	C-O	-6.09	1.17	1.24
1	B	98	PRO	CA-CB	-5.99	1.49	1.53
1	D	79	VAL	C-O	-5.99	1.17	1.24
1	C	248	PHE	C-O	-5.97	1.17	1.24
1	D	80	VAL	C-O	-5.96	1.17	1.24
1	A	36	VAL	C-O	-5.86	1.17	1.24
1	A	211	TRP	C-O	-5.81	1.17	1.24
1	A	252	THR	C-O	-5.80	1.16	1.24
1	B	269	SER	C-O	-5.76	1.16	1.23
1	B	192	THR	C-O	-5.76	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	VAL	C-O	-5.76	1.17	1.24
1	B	210	ASP	C-O	-5.76	1.16	1.24
1	D	279	ARG	C-O	-5.72	1.17	1.24
1	B	166	CYS	C-O	-5.72	1.17	1.24
1	C	247	SER	C-O	-5.66	1.16	1.23
1	A	37	VAL	C-O	-5.59	1.18	1.24
1	C	280	ALA	CA-CB	-5.59	1.44	1.53
1	C	305	ASN	C-O	-5.57	1.16	1.24
1	A	107	VAL	C-O	-5.49	1.18	1.24
1	A	88	VAL	C-O	-5.48	1.16	1.24
1	A	234	MET	C-O	-5.43	1.17	1.24
1	A	208	VAL	C-O	-5.40	1.17	1.24
1	A	324	ARG	C-O	-5.37	1.17	1.23
1	A	171	LEU	C-O	-5.36	1.17	1.24
1	A	38	ASP	C-O	-5.33	1.17	1.23
1	D	30	GLU	C-O	-5.32	1.17	1.24
1	C	135	ALA	CA-CB	-5.31	1.45	1.53
1	C	249	ARG	C-O	-5.27	1.17	1.24
1	A	35	ALA	C-O	-5.26	1.17	1.23
1	D	107	VAL	C-O	-5.26	1.18	1.24
1	A	255	VAL	C-O	-5.25	1.17	1.24
1	A	148	VAL	C-O	-5.24	1.17	1.23
1	D	134	SER	C-O	-5.23	1.17	1.24
1	A	86	LEU	C-O	-5.23	1.17	1.23
1	D	135	ALA	C-O	-5.22	1.17	1.24
1	D	37	VAL	C-O	-5.21	1.18	1.24
1	A	165	SER	C-O	-5.17	1.17	1.23
1	D	121	GLU	C-O	-5.17	1.17	1.24
1	A	35	ALA	CA-CB	-5.17	1.45	1.53
1	D	10	PHE	C-O	-5.12	1.17	1.24
1	D	127	GLY	C-O	-5.11	1.17	1.24
1	C	245	GLY	C-O	-5.06	1.17	1.23
1	D	324	ARG	C-O	-5.04	1.17	1.24
1	D	108	ILE	C-O	-5.01	1.18	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	MET	N-CA-C	-7.79	103.03	112.54
1	D	236	ILE	CA-C-N	6.27	126.75	119.47
1	D	236	ILE	C-N-CA	6.27	126.75	119.47
1	C	72	VAL	N-CA-C	5.54	117.86	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	283	THR	N-CA-C	5.37	116.68	108.30
1	C	288	ILE	N-CA-C	-5.09	107.18	111.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2733	0	2722	35	0
1	B	2733	0	2722	48	0
1	C	2733	0	2722	42	0
1	D	2733	0	2722	35	0
2	A	4	0	5	5	0
2	B	4	0	5	5	0
2	C	4	0	5	4	0
3	A	12	0	16	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	12	0	16	4	0
4	D	44	0	26	1	0
5	A	355	0	0	5	0
5	B	250	0	0	1	0
5	C	170	0	0	2	0
5	D	343	0	0	2	0
All	All	12142	0	10977	155	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 7.

All (155) 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:B:8:ASN:HD22	1:B:37:VAL:CG1	1.52	1.19
1:B:166:CYS:SG	2:B:360:ACM:H22	1.83	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:CYS:SG	2:C:360:ACM:H22	1.86	1.15
1:B:166:CYS:SG	2:B:360:ACM:C2	2.36	1.14
1:B:101:LYS:HE3	1:B:101:LYS:HA	1.32	1.10
1:B:8:ASN:HD22	1:B:37:VAL:HG13	1.16	1.09
1:C:129:ARG:HH11	1:C:129:ARG:HG3	0.96	1.07
1:C:129:ARG:HG3	1:C:129:ARG:NH1	1.61	1.02
1:B:8:ASN:HA	1:B:37:VAL:HG12	1.42	1.02
1:B:74:LYS:H	1:B:74:LYS:CD	1.74	1.00
1:B:42:ASP:OD1	1:B:44:GLU:HG2	1.61	1.00
1:B:8:ASN:ND2	1:B:37:VAL:CG1	2.25	0.99
1:B:101:LYS:HA	1:B:101:LYS:CE	1.91	0.99
1:B:8:ASN:HA	1:B:37:VAL:CG1	1.92	0.99
1:C:166:CYS:SG	2:C:360:ACM:C2	2.55	0.93
1:B:8:ASN:ND2	1:B:37:VAL:HG11	1.80	0.92
1:B:74:LYS:H	1:B:74:LYS:HD2	1.31	0.92
1:B:166:CYS:CB	2:B:360:ACM:H22	2.04	0.87
1:C:129:ARG:HH11	1:C:129:ARG:CG	1.83	0.86
1:B:166:CYS:SG	2:B:360:ACM:H23	2.15	0.86
1:B:74:LYS:CD	1:B:74:LYS:N	2.38	0.85
1:A:39:MET:HE3	1:A:39:MET:HA	1.60	0.83
1:B:19:GLN:HE22	1:B:50:MET:HG3	1.45	0.82
1:A:166:CYS:HB3	2:A:360:ACM:H22	1.61	0.82
1:C:129:ARG:NH1	1:C:129:ARG:CG	2.39	0.82
1:B:8:ASN:HD22	1:B:37:VAL:HG11	1.40	0.81
1:B:74:LYS:HD2	1:B:74:LYS:N	1.97	0.80
1:B:73:ALA:HB3	1:B:74:LYS:HD2	1.63	0.79
1:C:147:GLY:H	1:C:150:HIS:CD2	1.99	0.79
1:B:166:CYS:HB3	2:B:360:ACM:H22	1.64	0.79
1:B:8:ASN:ND2	1:B:37:VAL:HG13	1.95	0.78
1:A:50:MET:HE1	1:A:78:LEU:HD13	1.66	0.76
1:C:192:THR:HG23	1:C:247:SER:HB2	1.68	0.76
1:A:190:MET:HE1	1:A:258:VAL:HG22	1.67	0.75
1:C:8:ASN:HD22	1:C:37:VAL:HG13	1.54	0.72
1:C:190:MET:HE1	1:C:258:VAL:HG22	1.73	0.70
1:C:190:MET:HG2	1:C:229:ALA:HB2	1.74	0.70
1:C:166:CYS:CB	2:C:360:ACM:H22	2.23	0.69
1:D:147:GLY:H	1:D:150:HIS:CD2	2.11	0.68
1:D:37:VAL:HG22	4:D:360:NAD:H2A	1.75	0.68
2:A:360:ACM:H21	5:A:511:HOH:O	1.93	0.68
1:A:190:MET:HG2	1:A:229:ALA:HB2	1.78	0.66
1:A:166:CYS:SG	2:A:360:ACM:H23	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ASN:HD22	1:B:95:ALA:H	1.42	0.65
1:A:166:CYS:SG	2:A:360:ACM:C2	2.86	0.64
1:B:42:ASP:OD1	1:B:44:GLU:CG	2.43	0.64
1:C:181:GLU:OE2	1:C:279:ARG:NH2	2.30	0.64
1:A:147:GLY:H	1:A:150:HIS:CD2	2.15	0.64
1:A:200:GLN:HE21	1:A:249:ARG:HH11	1.47	0.63
1:D:147:GLY:H	1:D:150:HIS:HD2	1.47	0.62
1:D:171:LEU:HD13	1:D:232:VAL:HG21	1.81	0.62
1:B:15:ARG:O	1:B:19:GLN:HG2	2.00	0.62
1:B:101:LYS:HE3	1:B:101:LYS:CA	2.19	0.61
1:B:147:GLY:H	1:B:150:HIS:CD2	2.18	0.61
1:C:75:ASP:N	1:C:75:ASP:OD1	2.30	0.60
1:B:101:LYS:HA	1:B:101:LYS:NZ	2.15	0.60
1:D:21:LEU:HD11	1:D:31:ILE:CD1	2.32	0.60
1:A:239:THR:HB	1:A:243:LEU:HD13	1.84	0.59
1:D:91:GLN:NE2	1:D:96:ASP:OD2	2.35	0.59
1:A:200:GLN:NE2	1:A:249:ARG:HH11	2.00	0.59
1:C:74:LYS:HG2	1:C:75:ASP:H	1.69	0.58
1:C:166:CYS:HB3	2:C:360:ACM:H22	1.85	0.57
1:C:147:GLY:H	1:C:150:HIS:HD2	1.51	0.57
1:A:94:PRO:HA	1:A:97:LEU:HD22	1.87	0.57
1:C:8:ASN:HD22	1:C:37:VAL:CG1	2.18	0.56
1:D:129:ARG:HG3	3:D:362:GOL:O2	2.05	0.56
1:D:21:LEU:HD11	1:D:31:ILE:HD12	1.87	0.56
1:B:101:LYS:CE	1:B:101:LYS:CA	2.74	0.56
1:D:91:GLN:CD	1:D:96:ASP:OD2	2.49	0.56
1:A:328:LYS:NZ	5:A:534:HOH:O	2.38	0.56
1:C:8:ASN:HA	1:C:37:VAL:HG13	1.88	0.55
1:A:15:ARG:HG3	5:A:440:HOH:O	2.07	0.54
1:A:12:ARG:HG2	1:A:16:MET:HE2	1.87	0.54
1:A:39:MET:HE2	1:A:89:LYS:HZ1	1.71	0.54
1:A:166:CYS:CB	2:A:360:ACM:H22	2.35	0.54
1:B:74:LYS:H	1:B:74:LYS:HD3	1.65	0.53
1:B:91:GLN:HG3	1:B:97:LEU:HD13	1.90	0.53
1:C:124:LEU:HA	1:C:128:ALA:O	2.09	0.53
1:B:192:THR:HG21	1:B:333:TYR:OH	2.09	0.53
1:B:17:VAL:HG11	1:B:108:ILE:HD13	1.91	0.53
1:C:171:LEU:HD13	1:C:232:VAL:HG21	1.92	0.52
1:A:268:THR:OG1	1:A:269:SER:N	2.36	0.52
1:B:263:THR:HA	1:B:325:ARG:O	2.09	0.52
1:A:147:GLY:H	1:A:150:HIS:HD2	1.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:PRO:HG3	1:C:114:PHE:CE2	2.45	0.51
1:D:305:ASN:C	1:D:305:ASN:HD22	2.19	0.51
1:D:129:ARG:HD2	3:D:362:GOL:O1	2.10	0.51
1:C:37:VAL:HB	1:C:88:VAL:HG23	1.92	0.51
1:A:176:HIS:HE1	5:A:695:HOH:O	1.94	0.51
1:D:292:THR:HA	3:D:361:GOL:H31	1.94	0.50
1:C:19:GLN:HG3	1:C:59:PHE:CE1	2.47	0.50
1:A:151:HIS:HD2	5:A:698:HOH:O	1.95	0.49
1:A:244:THR:HG22	1:B:320:LEU:HG	1.95	0.49
1:D:129:ARG:HD2	3:D:362:GOL:C1	2.43	0.49
1:A:39:MET:HA	1:A:39:MET:CE	2.35	0.48
1:C:72:VAL:CG1	1:C:73:ALA:N	2.74	0.48
1:B:73:ALA:CB	1:B:74:LYS:HD2	2.37	0.48
1:B:348:ARG:HD2	5:B:749:HOH:O	2.14	0.48
1:D:219:VAL:HG22	1:D:219:VAL:O	2.14	0.48
1:B:44:GLU:CD	1:B:44:GLU:H	2.22	0.47
1:D:219:VAL:CG1	1:A:54:THR:HG21	2.44	0.47
1:D:321:PRO:O	1:D:322:LYS:HB2	2.13	0.47
1:B:50:MET:HE1	1:B:78:LEU:HD13	1.97	0.47
1:C:42:ASP:O	1:C:43:ALA:C	2.55	0.47
1:D:93:ASN:ND2	1:D:93:ASN:C	2.71	0.47
1:B:181:GLU:OE2	1:B:279:ARG:NH2	2.40	0.47
1:D:93:ASN:ND2	1:D:95:ALA:H	2.13	0.46
1:D:281:SER:HB2	1:D:289:LEU:O	2.15	0.46
1:D:219:VAL:HG13	1:A:54:THR:HG21	1.97	0.46
1:A:39:MET:HE2	1:A:89:LYS:NZ	2.30	0.46
1:C:180:LYS:N	1:C:180:LYS:HD2	2.32	0.45
1:D:2:PRO:HB2	1:D:32:ASP:HB2	1.98	0.45
1:C:122:GLY:HA2	1:C:125:ARG:HE	1.82	0.45
1:A:95:ALA:HB1	1:A:125:ARG:HG2	1.97	0.45
1:C:117:LYS:O	1:C:121:GLU:HG3	2.17	0.44
1:D:150:HIS:HE1	5:D:422:HOH:O	2.00	0.44
1:C:192:THR:HG23	1:C:247:SER:CB	2.45	0.44
1:C:196:TYR:HA	1:C:200:GLN:NE2	2.32	0.44
1:B:190:MET:HG3	1:B:258:VAL:HG13	1.99	0.44
1:D:21:LEU:HD11	1:D:31:ILE:HD13	1.99	0.44
1:C:176:HIS:HD2	5:C:401:HOH:O	2.00	0.43
1:A:33:VAL:O	1:A:83:HIS:HE1	2.00	0.43
1:C:97:LEU:HA	1:C:98:PRO:HD3	1.87	0.43
1:C:156:SER:OG	1:C:157:GLU:OE2	2.30	0.43
1:D:196:TYR:HA	1:D:200:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:LEU:HG	1:D:244:THR:HG22	1.99	0.43
1:B:352:SER:HA	1:B:355:ARG:HD2	2.00	0.43
1:C:12:ARG:HD3	1:B:204:ASP:O	2.18	0.43
1:B:196:TYR:HA	1:B:200:GLN:NE2	2.34	0.42
1:D:190:MET:HG3	1:D:258:VAL:HG13	2.01	0.42
1:C:171:LEU:HD22	1:C:175:VAL:HG23	2.01	0.42
1:B:40:ASN:HD21	1:B:42:ASP:HB3	1.84	0.42
1:B:91:GLN:CG	1:B:97:LEU:HD13	2.49	0.42
1:A:121:GLU:O	1:A:124:LEU:HB2	2.19	0.42
1:D:93:ASN:HD22	1:D:94:PRO:HD2	1.85	0.41
1:C:64:THR:HG22	1:C:65:THR:H	1.86	0.41
1:A:326:PHE:CE1	1:B:263:THR:HG23	2.56	0.41
5:C:1046:HOH:O	1:D:253:PRO:HD2	2.18	0.41
1:D:93:ASN:C	1:D:93:ASN:HD22	2.27	0.41
1:A:130:LYS:NZ	1:A:159:HIS:HD2	2.18	0.41
1:A:194:HIS:HB3	1:A:249:ARG:HD3	2.01	0.41
1:C:192:THR:CG2	1:C:247:SER:HB2	2.45	0.41
1:C:190:MET:HE2	1:C:191:THR:C	2.46	0.41
1:C:16:MET:HE2	1:C:16:MET:HB2	1.83	0.41
1:C:64:THR:HG22	1:C:65:THR:N	2.36	0.41
1:B:106:TYR:CD2	1:B:130:LYS:HB2	2.56	0.41
1:D:1:MET:HA	1:D:2:PRO:HD3	1.96	0.41
1:D:11:GLY:O	1:D:12:ARG:C	2.63	0.41
1:A:239:THR:HA	1:A:242:LYS:HD2	2.03	0.41
1:A:21:LEU:HD11	1:A:31:ILE:HG21	2.02	0.41
1:D:341:HIS:HE1	5:D:464:HOH:O	2.03	0.40
1:D:39:MET:HE3	1:D:39:MET:HA	2.03	0.40
1:D:233:GLY:O	1:D:237:PRO:HA	2.20	0.40
1:D:93:ASN:HD22	1:D:94:PRO:N	2.20	0.40
1:A:196:TYR:HA	1:A:200:GLN:NE2	2.36	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	357/359 (99%)	344 (96%)	12 (3%)	1 (0%)	36	25
1	B	357/359 (99%)	343 (96%)	13 (4%)	1 (0%)	36	25
1	C	357/359 (99%)	333 (93%)	23 (6%)	1 (0%)	36	25
1	D	357/359 (99%)	338 (95%)	18 (5%)	1 (0%)	36	25
All	All	1428/1436 (99%)	1358 (95%)	66 (5%)	4 (0%)	36	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	255	VAL
1	A	255	VAL
1	B	255	VAL
1	D	255	VAL

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	293/296 (99%)	279 (95%)	14 (5%)	23	11
1	B	293/296 (99%)	279 (95%)	14 (5%)	23	11
1	C	293/296 (99%)	283 (97%)	10 (3%)	32	20
1	D	293/296 (99%)	283 (97%)	10 (3%)	32	20
All	All	1172/1184 (99%)	1124 (96%)	48 (4%)	27	15

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4	LYS
1	C	16	MET
1	C	37	VAL
1	C	41	THR

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Mol	Chain	Res	Type
1	C	74	LYS
1	C	129	ARG
1	C	171	LEU
1	C	190	MET
1	C	305	ASN
1	C	355	ARG
1	D	21	LEU
1	D	37	VAL
1	D	39	MET
1	D	64	THR
1	D	88	VAL
1	D	92	ARG
1	D	102	LEU
1	D	157	GLU
1	D	171	LEU
1	D	305	ASN
1	A	15	ARG
1	A	40	ASN
1	A	58	LYS
1	A	74	LYS
1	A	97	LEU
1	A	102	LEU
1	A	124	LEU
1	A	125	ARG
1	A	157	GLU
1	A	190	MET
1	A	286	LYS
1	A	324	ARG
1	A	328	LYS
1	A	355	ARG
1	B	3	ILE
1	B	15	ARG
1	B	19	GLN
1	B	30	GLU
1	B	44	GLU
1	B	62	GLU
1	B	74	LYS
1	B	89	LYS
1	B	93	ASN
1	B	97	LEU
1	B	101	LYS
1	B	102	LEU

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Mol	Chain	Res	Type
1	B	243	LEU
1	B	353	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	ASN
1	C	83	HIS
1	C	150	HIS
1	C	154	ASN
1	C	159	HIS
1	C	176	HIS
1	C	200	GLN
1	C	240	GLN
1	C	305	ASN
1	C	349	HIS
1	D	49	GLN
1	D	83	HIS
1	D	93	ASN
1	D	150	HIS
1	D	159	HIS
1	D	186	GLN
1	D	200	GLN
1	D	303	ASN
1	D	305	ASN
1	D	341	HIS
1	A	8	ASN
1	A	19	GLN
1	A	83	HIS
1	A	93	ASN
1	A	150	HIS
1	A	151	HIS
1	A	159	HIS
1	A	176	HIS
1	A	200	GLN
1	B	8	ASN
1	B	19	GLN
1	B	93	ASN
1	B	150	HIS
1	B	159	HIS
1	B	200	GLN
1	B	305	ASN

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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	361	-	5,5,5	0.37	0	5,5,5	0.36	0
2	ACM	A	360	-	3,3,3	0.59	0	3,3,3	0.26	0
3	GOL	A	362	-	5,5,5	0.27	0	5,5,5	0.52	0
2	ACM	B	360	-	3,3,3	1.64	1 (33%)	3,3,3	0.35	0
4	NAD	D	360	-	46,48,48	1.48	6 (13%)	64,73,73	1.59	9 (14%)
3	GOL	B	361	-	5,5,5	0.33	0	5,5,5	0.55	0
3	GOL	C	361	-	5,5,5	0.39	0	5,5,5	0.43	0
3	GOL	D	361	-	5,5,5	0.38	0	5,5,5	0.32	0
2	ACM	C	360	-	3,3,3	1.52	1 (33%)	3,3,3	1.02	0
3	GOL	D	362	-	5,5,5	0.74	0	5,5,5	0.73	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
3	GOL	A	361	-	-	0/4/4/4	-
3	GOL	A	362	-	-	0/4/4/4	-
4	NAD	D	360	-	-	8/30/62/62	0/5/5/5
3	GOL	B	361	-	-	2/4/4/4	-
3	GOL	C	361	-	-	0/4/4/4	-
3	GOL	D	361	-	-	2/4/4/4	-
3	GOL	D	362	-	-	4/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	360	NAD	C2N-N1N	5.70	1.41	1.35
4	D	360	NAD	C3N-C7N	3.82	1.56	1.50
4	D	360	NAD	PA-O3	2.87	1.62	1.59
4	D	360	NAD	C5A-N7A	-2.87	1.33	1.39
2	B	360	ACM	O-C1	-2.61	1.19	1.24
2	C	360	ACM	O-C1	-2.30	1.19	1.24
4	D	360	NAD	C6N-N1N	2.17	1.40	1.35
4	D	360	NAD	C4A-N9A	-2.02	1.33	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	360	NAD	N3A-C2A-N1A	-5.26	120.62	128.58
4	D	360	NAD	C5A-C4A-N3A	-4.74	120.19	126.72
4	D	360	NAD	C2A-N3A-C4A	3.67	120.80	111.83
4	D	360	NAD	N9A-C8A-N7A	-3.67	108.73	113.94
4	D	360	NAD	N3A-C4A-N9A	3.21	132.62	127.17
4	D	360	NAD	C5A-N7A-C8A	2.82	107.88	103.45
4	D	360	NAD	C4A-N9A-C8A	2.60	108.47	105.74
4	D	360	NAD	C4A-C5A-N7A	-2.50	107.73	110.58
4	D	360	NAD	O2A-PA-O3	2.05	112.80	107.27

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	362	GOL	O1-C1-C2-C3
3	D	362	GOL	C1-C2-C3-O3
4	D	360	NAD	C5B-O5B-PA-O1A
4	D	360	NAD	O4D-C1D-N1N-C2N

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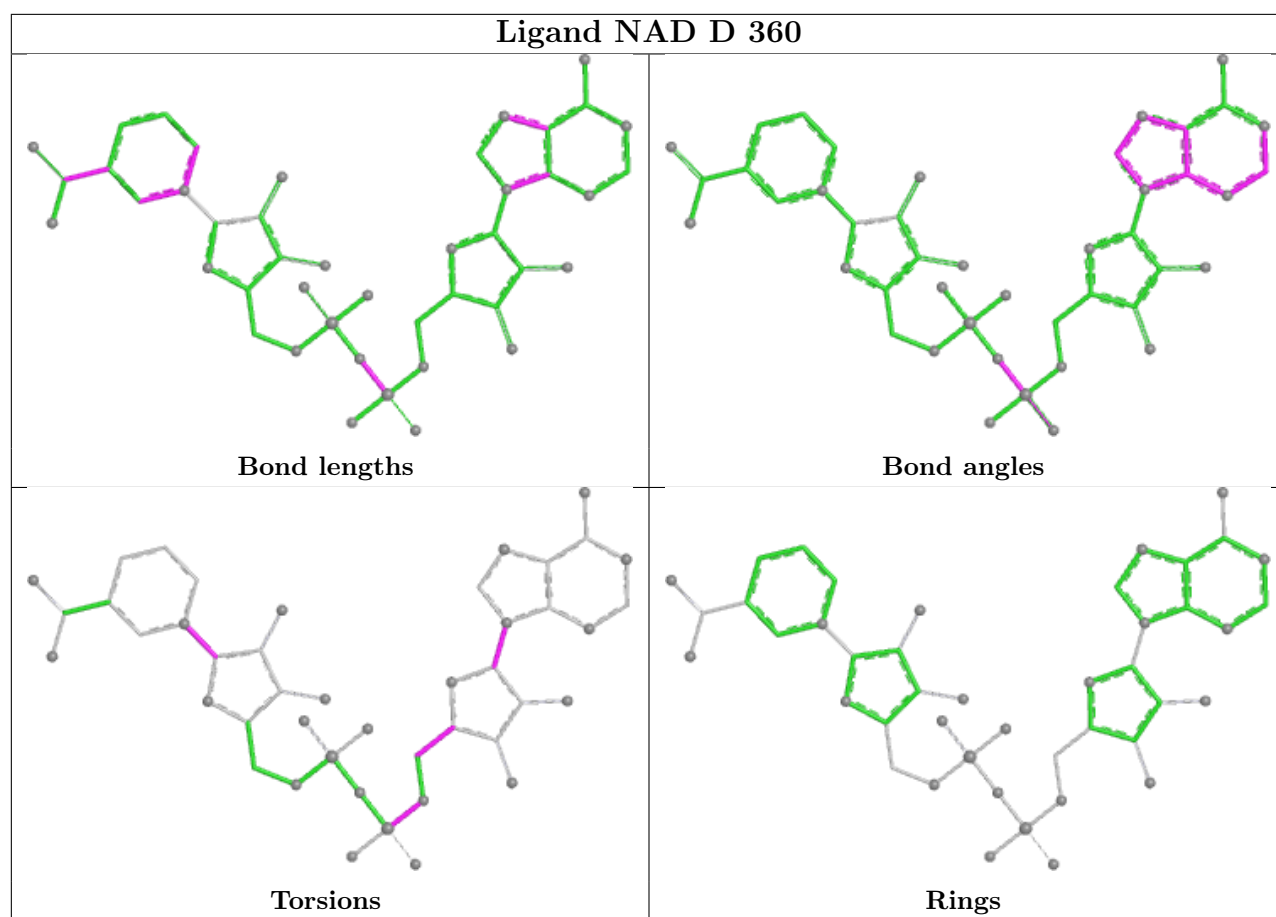
Mol	Chain	Res	Type	Atoms
4	D	360	NAD	C2D-C1D-N1N-C2N
4	D	360	NAD	C2D-C1D-N1N-C6N
3	D	361	GOL	O1-C1-C2-C3
3	B	361	GOL	C1-C2-C3-O3
3	D	362	GOL	O1-C1-C2-O2
3	D	362	GOL	O2-C2-C3-O3
3	D	361	GOL	O1-C1-C2-O2
3	B	361	GOL	O2-C2-C3-O3
4	D	360	NAD	C2B-C1B-N9A-C8A
4	D	360	NAD	O4D-C1D-N1N-C6N
4	D	360	NAD	O4B-C4B-C5B-O5B
4	D	360	NAD	C2B-C1B-N9A-C4A

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	360	ACM	5	0
2	B	360	ACM	5	0
4	D	360	NAD	1	0
3	D	361	GOL	1	0
2	C	360	ACM	4	0
3	D	362	GOL	3	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	359/359 (100%)	0.01	8 (2%) 62 62	14, 24, 40, 60	2 (0%)
1	B	359/359 (100%)	0.86	68 (18%) 3 2	13, 32, 62, 80	1 (0%)
1	C	359/359 (100%)	1.46	123 (34%) 1 1	2, 35, 83, 96	2 (0%)
1	D	359/359 (100%)	0.10	9 (2%) 58 58	16, 25, 40, 58	2 (0%)
All	All	1436/1436 (100%)	0.61	208 (14%) 6 5	2, 27, 68, 96	7 (0%)

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	GLU	24.4
1	C	104	VAL	6.4
1	C	37	VAL	6.2
1	C	97	LEU	5.8
1	C	124	LEU	5.8
1	C	99	TRP	5.7
1	C	107	VAL	5.7
1	C	95	ALA	5.6
1	C	356	SER	5.6
1	C	116	ALA	5.4
1	B	357	ALA	5.4
1	C	352	SER	5.2
1	C	3	ILE	5.2
1	C	2	PRO	5.1
1	D	359	LEU	5.1
1	C	98	PRO	4.9
1	C	103	GLY	4.9
1	C	122	GLY	4.9
1	C	72	VAL	4.9
1	C	351	ALA	4.8
1	C	86	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	102	LEU	4.7
1	B	358	ARG	4.6
1	A	359	LEU	4.6
1	C	79	VAL	4.4
1	C	153	TYR	4.4
1	C	154	ASN	4.4
1	C	73	ALA	4.4
1	C	27	LEU	4.3
1	C	357	ALA	4.3
1	C	126	GLY	4.3
1	C	155	PRO	4.2
1	C	106	TYR	4.1
1	D	96	ASP	4.1
1	C	128	ALA	4.0
1	C	127	GLY	3.9
1	B	88	VAL	3.9
1	C	123	HIS	3.9
1	C	31	ILE	3.9
1	C	21	LEU	3.8
1	C	1	MET	3.8
1	B	119	ALA	3.8
1	B	118	ALA	3.8
1	B	3	ILE	3.7
1	B	73	ALA	3.7
1	C	125	ARG	3.7
1	B	95	ALA	3.7
1	B	1	MET	3.7
1	B	72	VAL	3.7
1	C	70	PRO	3.7
1	C	359	LEU	3.6
1	C	4	LYS	3.6
1	B	70	PRO	3.6
1	C	130	LYS	3.6
1	B	124	LEU	3.6
1	C	9	GLY	3.5
1	C	66	THR	3.5
1	C	114	PHE	3.5
1	C	119	ALA	3.4
1	C	88	VAL	3.4
1	C	105	GLU	3.4
1	C	141	ALA	3.4
1	B	69	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	67	LYS	3.4
1	C	131	VAL	3.4
1	B	102	LEU	3.4
1	C	94	PRO	3.4
1	C	158	HIS	3.3
1	C	355	ARG	3.3
1	C	35	ALA	3.3
1	B	63	VAL	3.3
1	B	359	LEU	3.3
1	C	69	SER	3.3
1	C	138	SER	3.3
1	B	79	VAL	3.2
1	B	225	THR	3.2
1	C	113	LEU	3.2
1	C	85	ILE	3.1
1	A	1	MET	3.1
1	B	129	ARG	3.1
1	D	1	MET	3.1
1	C	115	THR	3.1
1	C	34	VAL	3.1
1	C	38	ASP	3.1
1	B	46	PHE	3.1
1	B	114	PHE	3.1
1	C	5	VAL	3.0
1	B	93	ASN	3.0
1	C	36	VAL	3.0
1	D	37	VAL	3.0
1	C	46	PHE	3.0
1	B	66	THR	3.0
1	B	115	THR	3.0
1	C	139	GLY	2.9
1	C	354	ASP	2.9
1	C	199	THR	2.9
1	C	87	CYS	2.9
1	B	13	ILE	2.9
1	C	16	MET	2.9
1	B	37	VAL	2.9
1	C	41	THR	2.9
1	B	42	ASP	2.9
1	D	72	VAL	2.8
1	C	26	LEU	2.8
1	C	13	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	129	ARG	2.8
1	B	85	ILE	2.8
1	C	80	VAL	2.8
1	B	116	ALA	2.8
1	C	83	HIS	2.8
1	B	131	VAL	2.8
1	C	23	GLU	2.7
1	C	93	ASN	2.7
1	B	36	VAL	2.7
1	C	100	GLY	2.6
1	B	351	ALA	2.6
1	C	39	MET	2.6
1	B	94	PRO	2.6
1	C	347	VAL	2.6
1	B	356	SER	2.6
1	B	98	PRO	2.6
1	B	113	LEU	2.6
1	C	78	LEU	2.6
1	C	11	GLY	2.6
1	C	225	THR	2.6
1	B	29	THR	2.6
1	C	159	HIS	2.5
1	C	117	LYS	2.5
1	C	133	ILE	2.5
1	C	32	ASP	2.5
1	C	67	LYS	2.5
1	C	74	LYS	2.5
1	B	205	GLY	2.5
1	C	90	ALA	2.5
1	C	118	ALA	2.5
1	C	29	THR	2.5
1	C	160	VAL	2.5
1	B	208	VAL	2.5
1	B	61	TYR	2.5
1	C	6	GLY	2.5
1	C	140	GLY	2.5
1	C	108	ILE	2.5
1	C	156	SER	2.5
1	C	120	ALA	2.5
1	C	33	VAL	2.5
1	B	53	ASP	2.5
1	B	107	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	137	ALA	2.4
1	B	355	ARG	2.4
1	C	28	GLY	2.4
1	B	91	GLN	2.4
1	B	16	MET	2.4
1	C	132	VAL	2.4
1	B	41	THR	2.4
1	B	83	HIS	2.4
1	B	39	MET	2.4
1	C	53	ASP	2.3
1	C	20	ALA	2.3
1	C	43	ALA	2.3
1	C	234	MET	2.3
1	B	8	ASN	2.3
1	B	43	ALA	2.3
1	C	7	ILE	2.3
1	C	65	THR	2.3
1	B	71	SER	2.3
1	B	337	TRP	2.2
1	C	205	GLY	2.2
1	A	73	ALA	2.2
1	B	112	GLY	2.2
1	C	208	VAL	2.2
1	C	358	ARG	2.2
1	C	144	LEU	2.2
1	B	120	ALA	2.2
1	C	40	ASN	2.2
1	C	151	HIS	2.2
1	C	111	THR	2.2
1	D	122	GLY	2.2
1	C	59	PHE	2.2
1	B	30	GLU	2.2
1	C	344	VAL	2.2
1	C	64	THR	2.2
1	B	77	THR	2.2
1	B	97	LEU	2.2
1	A	13	ILE	2.1
1	B	99	TRP	2.1
1	B	76	ASP	2.1
1	B	80	VAL	2.1
1	B	104	VAL	2.1
1	B	103	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	87	CYS	2.1
1	C	12	ARG	2.1
1	A	355	ARG	2.1
1	D	90	ALA	2.1
1	C	92	ARG	2.1
1	C	161	VAL	2.1
1	B	9	GLY	2.1
1	D	92	ARG	2.1
1	C	353	LYS	2.1
1	B	44	GLU	2.1
1	D	206	VAL	2.1
1	A	358	ARG	2.1
1	A	337	TRP	2.0
1	A	62	GLU	2.0
1	C	18	PHE	2.0
1	C	91	GLN	2.0
1	B	126	GLY	2.0
1	C	84	ARG	2.0
1	B	206	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

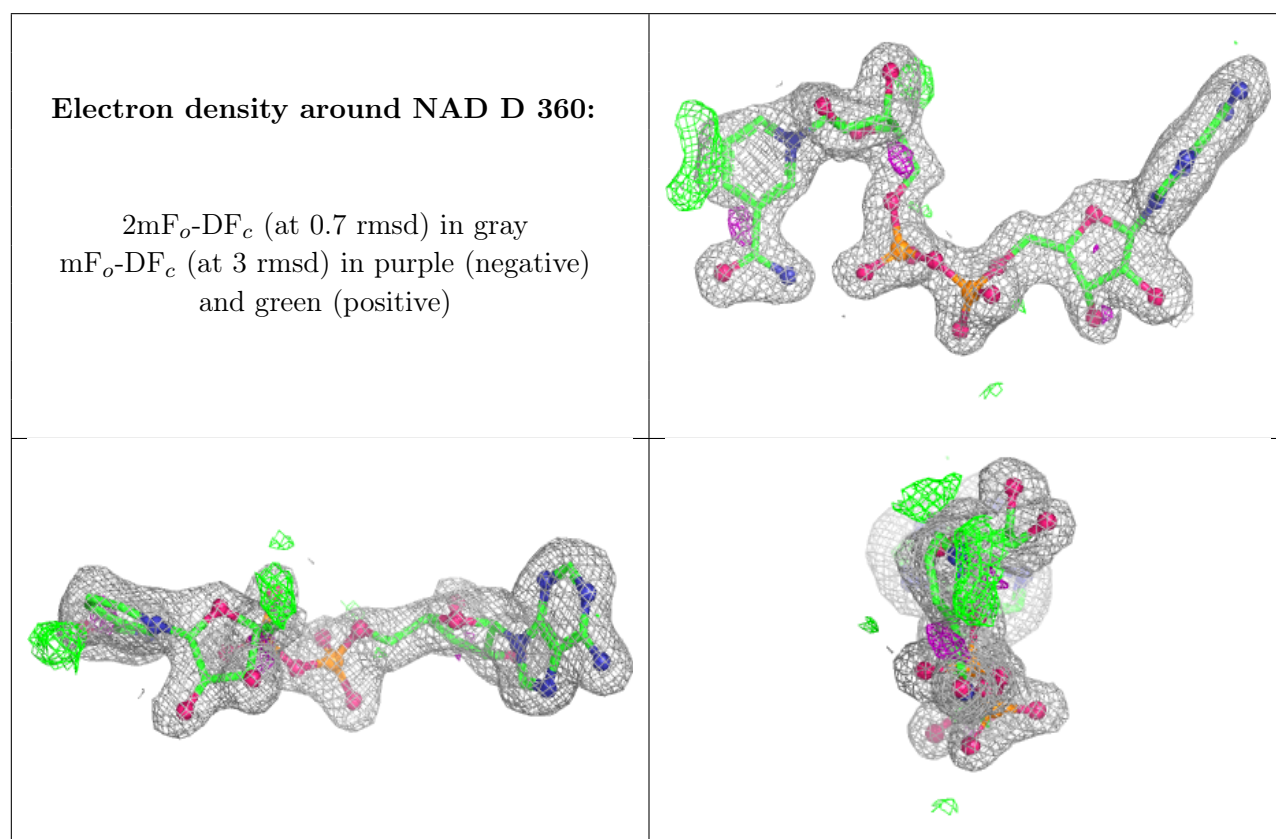
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACM	A	360	4/4	0.62	0.23	33,35,37,40	0
3	GOL	D	362	6/6	0.77	0.12	34,39,42,47	0
3	GOL	A	362	6/6	0.79	0.14	33,37,42,45	0
3	GOL	A	361	6/6	0.80	0.12	33,36,43,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	361	6/6	0.84	0.12	31,37,43,45	0
2	ACM	C	360	4/4	0.85	0.14	32,37,39,41	0
3	GOL	B	361	6/6	0.87	0.10	31,35,37,40	0
2	ACM	B	360	4/4	0.88	0.11	33,35,37,37	0
3	GOL	D	361	6/6	0.88	0.09	32,35,40,46	0
4	NAD	D	360	44/44	0.92	0.09	17,30,34,35	2

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.



6.5 Other polymers ⓘ

There are no such residues in this entry.