



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:06 PM UTC

PDB ID : 3ZW9 / pdb_00003zw9
Title : CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE 1 (RPMFE1) COMPLEXED WITH (2S,3S)-3-HYDROXY-2-METHYLBUTANOYL-COA
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Deposited on : 2011-07-28
Resolution : 2.90 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

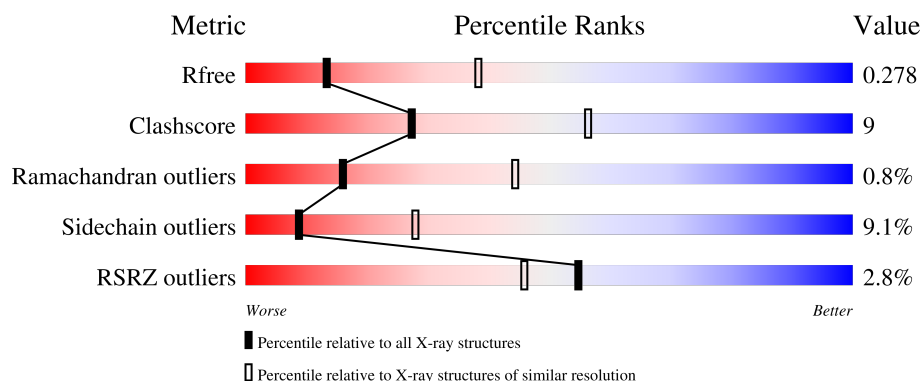
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	742	3% 75% 20% ..
1	B	742	2% 70% 25% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11399 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 PEROXISOMAL BIFUNCTIONAL ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	0	0
			5544	3542	971	1008	23			
1	B	719	Total	C	N	O	S	0	1	0
			5528	3534	968	1003	23			

There are 40 discrepancies between the modelled and reference sequences:

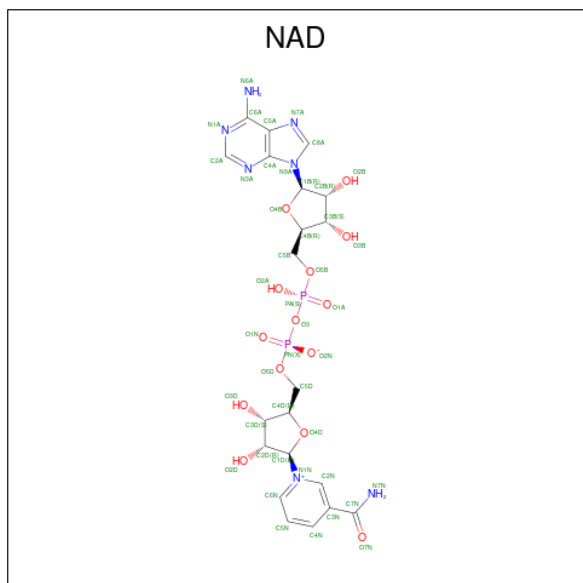
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P07896
A	-18	GLY	-	expression tag	UNP P07896
A	-17	SER	-	expression tag	UNP P07896
A	-16	SER	-	expression tag	UNP P07896
A	-15	HIS	-	expression tag	UNP P07896
A	-14	HIS	-	expression tag	UNP P07896
A	-13	HIS	-	expression tag	UNP P07896
A	-12	HIS	-	expression tag	UNP P07896
A	-11	HIS	-	expression tag	UNP P07896
A	-10	HIS	-	expression tag	UNP P07896
A	-9	SER	-	expression tag	UNP P07896
A	-8	SER	-	expression tag	UNP P07896
A	-7	GLY	-	expression tag	UNP P07896
A	-6	LEU	-	expression tag	UNP P07896
A	-5	VAL	-	expression tag	UNP P07896
A	-4	PRO	-	expression tag	UNP P07896
A	-3	ARG	-	expression tag	UNP P07896
A	-2	GLY	-	expression tag	UNP P07896
A	-1	SER	-	expression tag	UNP P07896
A	0	HIS	-	expression tag	UNP P07896
B	-19	MET	-	expression tag	UNP P07896
B	-18	GLY	-	expression tag	UNP P07896
B	-17	SER	-	expression tag	UNP P07896
B	-16	SER	-	expression tag	UNP P07896
B	-15	HIS	-	expression tag	UNP P07896

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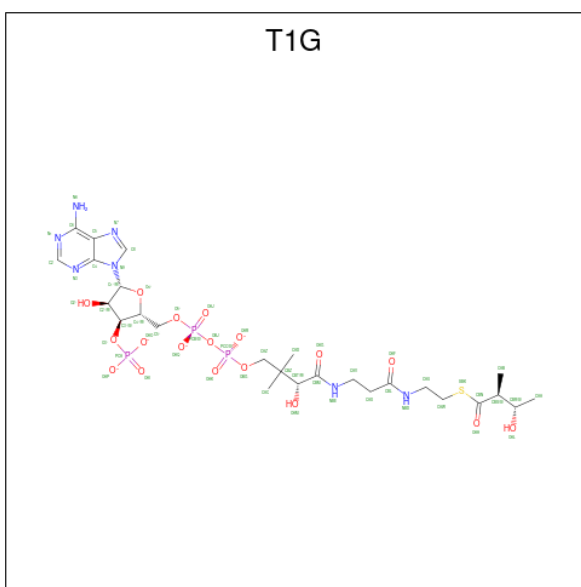
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P07896
B	-13	HIS	-	expression tag	UNP P07896
B	-12	HIS	-	expression tag	UNP P07896
B	-11	HIS	-	expression tag	UNP P07896
B	-10	HIS	-	expression tag	UNP P07896
B	-9	SER	-	expression tag	UNP P07896
B	-8	SER	-	expression tag	UNP P07896
B	-7	GLY	-	expression tag	UNP P07896
B	-6	LEU	-	expression tag	UNP P07896
B	-5	VAL	-	expression tag	UNP P07896
B	-4	PRO	-	expression tag	UNP P07896
B	-3	ARG	-	expression tag	UNP P07896
B	-2	GLY	-	expression tag	UNP P07896
B	-1	SER	-	expression tag	UNP P07896
B	0	HIS	-	expression tag	UNP P07896

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



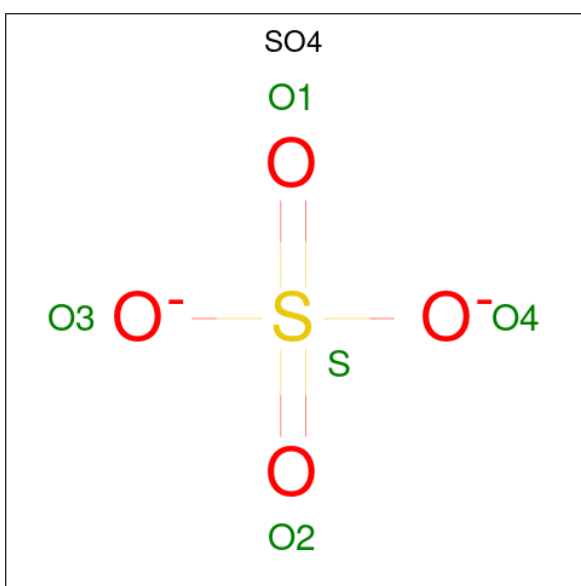
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is (2S,3S)-3-HYDROXY-2-METHYLBUTANOYL-COA (CCD ID: T1G) (formula: $C_{26}H_{40}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			55	26	7	18	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			55	26	7	18	3	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total	O	0	0
			66	66		
5	B	48	Total	O	0	0
			48	48		

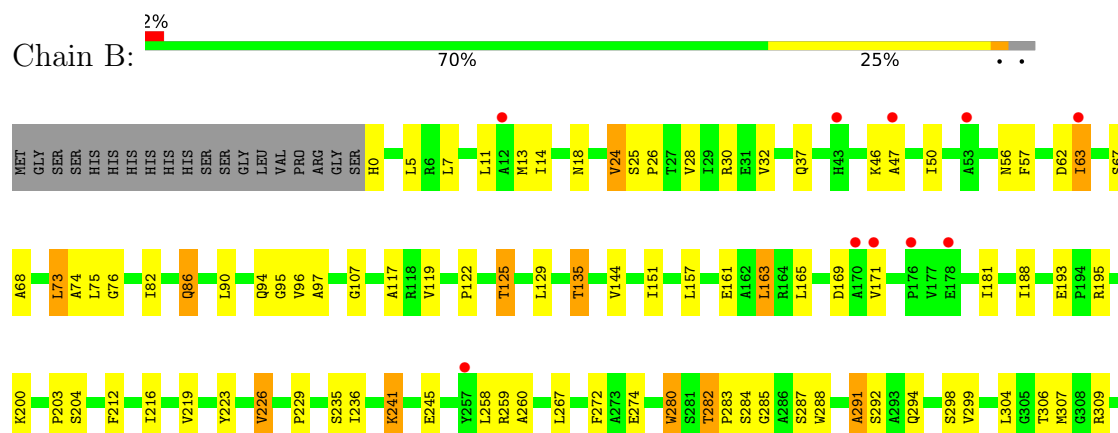
3 Residue-property plots

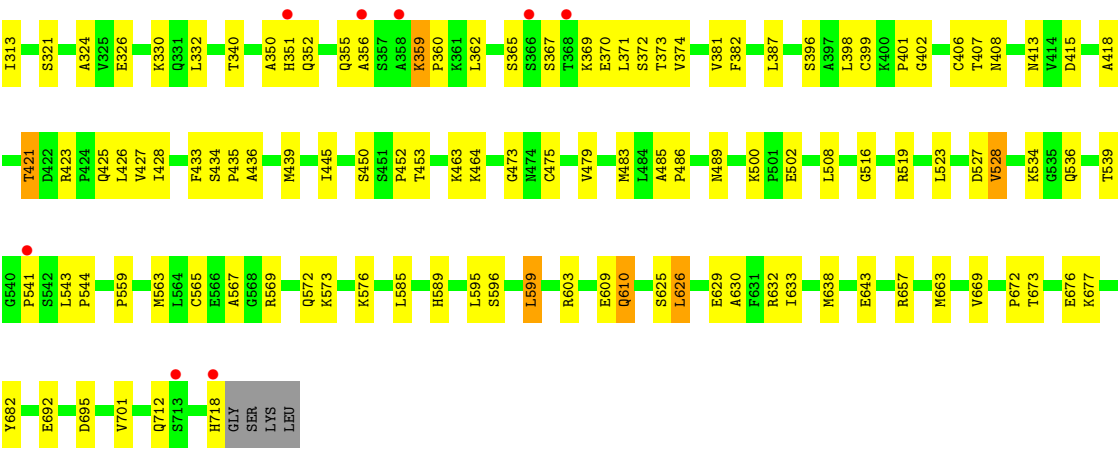
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME



• Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.59Å 126.65Å 225.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.90 100.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (100.00-2.90) 100.0 (100.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.228 , 0.287 0.222 , 0.278	Depositor DCC
R_{free} test set	2147 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11399	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: T1G, SO4, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.84	2/5672 (0.0%)	1.02	13/7684 (0.2%)
1	B	0.82	0/5660	1.03	17/7669 (0.2%)
All	All	0.83	2/11332 (0.0%)	1.03	30/15353 (0.2%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	VAL	CA-CB	5.31	1.60	1.54
1	A	438	VAL	CA-CB	5.29	1.59	1.55

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	LEU	N-CA-C	8.49	120.16	111.07
1	B	18	ASN	CA-C-N	6.80	124.62	119.66
1	B	18	ASN	C-N-CA	6.80	124.62	119.66
1	B	669	VAL	N-CA-C	-6.45	103.97	111.00
1	B	193	GLU	CA-C-N	-6.44	112.97	120.12
1	B	193	GLU	C-N-CA	-6.44	112.97	120.12
1	A	200	LYS	CA-C-N	-5.72	114.37	120.03
1	A	200	LYS	C-N-CA	-5.72	114.37	120.03
1	B	200	LYS	CA-C-N	-5.72	114.72	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	LYS	C-N-CA	-5.72	114.72	120.21
1	B	528	VAL	N-CA-C	5.70	116.47	110.72
1	B	625	SER	N-CA-C	-5.68	104.99	111.07
1	A	18	ASN	CA-C-N	5.65	126.20	120.38
1	A	18	ASN	C-N-CA	5.65	126.20	120.38
1	A	241	LYS	N-CA-C	5.64	119.68	112.34
1	B	291	ALA	N-CA-C	5.60	117.55	110.33
1	A	226	VAL	CB-CA-C	5.48	117.59	110.96
1	A	366	SER	N-CA-C	-5.29	106.82	113.28
1	B	516	GLY	CA-C-N	5.20	125.25	119.32
1	B	516	GLY	C-N-CA	5.20	125.25	119.32
1	B	76	GLY	N-CA-C	-5.12	106.56	112.50
1	A	543	LEU	CA-C-N	5.08	125.61	120.38
1	A	543	LEU	C-N-CA	5.08	125.61	120.38
1	B	24	VAL	CB-CA-C	-5.07	104.56	111.15
1	B	541	PRO	N-CA-C	-5.05	108.04	114.35
1	B	280	TRP	N-CA-C	5.03	117.17	110.53
1	B	241	LYS	N-CA-C	5.02	118.50	112.38
1	A	516	GLY	CA-C-N	5.01	124.45	119.24
1	A	516	GLY	C-N-CA	5.01	124.45	119.24
1	A	76	GLY	N-CA-C	-5.00	106.37	112.77

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	GLY	Peptide

5.2 Too-close contacts [i](#)

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	5544	0	5647	87	0
1	B	5528	0	5633	121	0
2	A	44	0	26	2	0
2	B	44	0	26	2	0
3	A	55	0	40	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	55	0	40	5	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
5	A	66	0	0	8	0
5	B	48	0	0	9	0
All	All	11399	0	11412	207	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 (207) 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:A:73:LEU:HD11	1:A:252:GLU:HG3	1.30	1.13
1:B:73:LEU:H	1:B:73:LEU:HD12	1.04	1.06
1:B:486:PRO:HA	1:B:489[A]:ASN:ND2	1.80	0.96
1:B:73:LEU:HD12	1:B:73:LEU:N	1.85	0.92
1:A:135:THR:HG21	1:A:235:SER:OG	1.70	0.91
1:A:597:THR:HG23	1:B:382:PHE:CZ	2.05	0.91
1:B:73:LEU:H	1:B:73:LEU:CD1	1.87	0.88
1:B:350:ALA:HB1	1:B:355:GLN:HB2	1.54	0.88
1:B:86:GLN:HE21	1:B:86:GLN:HA	1.36	0.88
1:B:672:PRO:HG3	5:B:2047:HOH:O	1.74	0.86
3:B:1721:T1G:OAJ	3:B:1721:T1G:H3'	1.78	0.84
1:A:396:SER:HB2	1:A:421:THR:HG22	1.61	0.83
1:A:122:PRO:O	1:A:125:THR:HB	1.79	0.82
1:B:396:SER:HB2	1:B:421:THR:HG22	1.60	0.82
1:A:274:GLU:OE2	1:A:657:ARG:NH2	2.15	0.79
1:A:86:GLN:HE21	1:A:86:GLN:HA	1.48	0.78
1:A:597:THR:CG2	1:B:382:PHE:CZ	2.67	0.77
1:A:73:LEU:HD11	1:A:252:GLU:CG	2.15	0.75
1:B:63:ILE:HD12	1:B:272:PHE:HE1	1.53	0.74
1:A:100:GLY:N	3:A:1722:T1G:OAH	2.21	0.73
1:B:135:THR:HG21	1:B:235:SER:OG	1.90	0.72
1:A:597:THR:HG23	1:B:382:PHE:HZ	1.48	0.71
1:A:597:THR:CG2	1:B:382:PHE:HZ	2.02	0.71
1:B:519:ARG:HD3	1:B:589:HIS:CE1	2.25	0.71
1:B:24:VAL:HG11	1:B:75:LEU:HD13	1.73	0.69
1:B:486:PRO:HA	1:B:489[A]:ASN:HD22	1.55	0.69
1:B:63:ILE:HD12	1:B:272:PHE:CE1	2.29	0.68
1:A:382:PHE:CD2	2:A:1721:NAD:H8A	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:HD23	5:A:2039:HOH:O	1.94	0.67
1:A:370:GLU:O	5:A:2029:HOH:O	2.14	0.66
1:B:274:GLU:OE2	1:B:657:ARG:NH2	2.29	0.66
1:B:122:PRO:O	1:B:125:THR:HB	1.96	0.66
1:A:123:GLU:OE2	3:A:1722:T1G:OAH	2.13	0.65
1:A:304:LEU:HD11	1:A:324:ALA:HB1	1.79	0.64
1:B:129:LEU:HD12	1:B:129:LEU:C	2.24	0.63
1:B:74:ALA:HA	5:B:2011:HOH:O	1.99	0.62
1:A:519:ARG:HD3	1:A:589:HIS:CE1	2.35	0.62
1:B:82:ILE:HG22	1:B:107:GLY:O	1.99	0.62
1:B:73:LEU:N	1:B:73:LEU:CD1	2.53	0.62
1:B:67:SER:O	1:B:259:ARG:NH2	2.33	0.61
1:B:63:ILE:HG12	3:B:1721:T1G:N1	2.15	0.61
1:A:67:SER:HB3	1:A:70:THR:OG1	2.02	0.60
1:B:97:ALA:HB3	1:B:119:VAL:HG12	1.82	0.60
1:B:304:LEU:HD11	1:B:324:ALA:HB1	1.83	0.60
1:B:382:PHE:HB2	1:B:387:LEU:HD23	1.84	0.60
1:B:267:LEU:HD23	1:B:657:ARG:HG2	1.84	0.59
1:B:519:ARG:HD3	1:B:589:HIS:NE2	2.19	0.58
1:A:305:GLY:HA3	2:A:1721:NAD:O5B	2.04	0.57
1:A:494:LEU:HD13	1:A:618:ILE:HG12	1.86	0.57
1:A:307:MET:SD	1:A:434:SER:HB3	2.44	0.57
1:A:365:SER:HB2	1:A:370:GLU:OE2	2.05	0.57
1:A:135:THR:HG21	1:A:235:SER:HG	1.70	0.56
1:A:382:PHE:HB2	1:A:387:LEU:HD23	1.86	0.56
1:B:475:CYS:HB3	1:B:638:MET:SD	2.45	0.56
1:B:475:CYS:SG	1:B:638:MET:HG3	2.45	0.56
1:A:169:ASP:CG	1:A:195:ARG:HH22	2.14	0.56
1:A:401:PRO:HA	1:A:423:ARG:HH12	1.71	0.56
1:A:84:ARG:HD2	5:A:2010:HOH:O	2.06	0.56
1:B:309:ARG:O	1:B:313:ILE:HD12	2.05	0.56
1:B:280:TRP:O	1:B:288:TRP:HD1	1.88	0.56
1:A:73:LEU:HD13	1:A:256:MET:HE3	1.89	0.55
1:B:643:GLU:OE1	1:B:643:GLU:N	2.32	0.55
1:A:97:ALA:HB3	1:A:119:VAL:HG12	1.88	0.55
1:B:485:ALA:HB3	1:B:486:PRO:HD3	1.88	0.55
1:B:682:TYR:CE2	1:B:692:GLU:HG3	2.42	0.55
1:B:633:ILE:HG23	1:B:638:MET:HB2	1.89	0.54
1:B:712:GLN:HA	1:B:712:GLN:OE1	2.07	0.54
1:A:368:THR:HG21	5:A:2031:HOH:O	2.07	0.54
1:A:418:ALA:O	1:A:421:THR:OG1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ALA:O	1:B:421:THR:OG1	2.26	0.53
1:B:46:LYS:HB2	1:B:188:ILE:HD11	1.90	0.53
1:B:63:ILE:HB	1:B:272:PHE:HZ	1.72	0.53
1:A:500:LYS:HB3	1:A:502:GLU:OE1	2.09	0.53
1:B:595:LEU:O	1:B:599:LEU:HB2	2.08	0.53
1:B:473:GLY:HA3	1:B:638:MET:SD	2.49	0.53
1:A:46:LYS:HB2	1:A:188:ILE:HD11	1.92	0.52
1:A:565:CYS:C	1:A:567:ALA:H	2.17	0.52
1:B:26:PRO:HD3	5:B:2001:HOH:O	2.08	0.52
1:B:282:THR:HG22	1:B:283:PRO:HD2	1.92	0.52
1:B:500:LYS:HB3	1:B:502:GLU:OE1	2.09	0.52
1:B:62:ASP:HB3	5:B:2003:HOH:O	2.08	0.52
1:A:519:ARG:HD3	1:A:589:HIS:NE2	2.24	0.52
1:B:372:SER:HA	1:B:399:CYS:HA	1.90	0.52
1:A:367:SER:HA	5:A:2030:HOH:O	2.09	0.52
1:B:534:LYS:HG2	1:B:539:THR:HG23	1.91	0.52
1:B:63:ILE:HG12	3:B:1721:T1G:C6	2.41	0.51
1:A:86:GLN:HE21	1:A:86:GLN:CA	2.22	0.51
1:B:413:ASN:OD1	1:B:415:ASP:HB2	2.10	0.51
1:B:86:GLN:HA	1:B:86:GLN:NE2	2.15	0.51
1:B:95:GLY:O	1:B:117:ALA:HA	2.11	0.51
1:B:7:LEU:HD21	1:B:181:ILE:HD11	1.93	0.51
1:B:663:MET:HA	1:B:663:MET:HE2	1.92	0.51
1:A:73:LEU:HD21	1:A:252:GLU:CD	2.35	0.50
1:A:95:GLY:O	1:A:117:ALA:HA	2.11	0.50
1:A:283:PRO:O	1:A:284:SER:CB	2.58	0.50
1:A:256:MET:HE2	1:A:259:ARG:HH12	1.77	0.50
1:A:283:PRO:O	1:A:284:SER:HB3	2.12	0.50
1:A:607:HIS:ND1	5:A:2049:HOH:O	2.35	0.50
1:B:241:LYS:HD2	5:B:2023:HOH:O	2.12	0.50
1:B:479:VAL:HG22	1:B:633:ILE:HG21	1.94	0.50
1:A:51:CYS:HB3	1:A:92:ALA:HB3	1.94	0.50
1:A:401:PRO:HA	1:A:423:ARG:NH1	2.26	0.49
1:A:663:MET:HA	1:A:663:MET:HE2	1.95	0.49
1:B:226:VAL:O	1:B:229:PRO:HD2	2.12	0.49
1:B:565:CYS:C	1:B:567:ALA:H	2.20	0.49
1:B:673:THR:O	1:B:677:LYS:HG2	2.13	0.49
1:B:86:GLN:HE21	1:B:86:GLN:CA	2.16	0.49
1:B:151:ILE:HD12	1:B:236:ILE:HD11	1.94	0.49
1:B:291:ALA:HB2	1:B:452:PRO:HB3	1.94	0.49
1:B:169:ASP:CG	1:B:195:ARG:HH22	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HG21	1:A:75:LEU:HD13	1.95	0.48
1:A:350:ALA:HB1	1:A:356:ALA:HB3	1.94	0.48
1:A:169:ASP:OD2	1:A:195:ARG:NH2	2.47	0.48
1:A:274:GLU:CD	1:A:657:ARG:NH2	2.72	0.47
1:A:129:LEU:C	1:A:129:LEU:HD12	2.40	0.47
1:A:445:ILE:HD12	1:A:445:ILE:N	2.29	0.47
1:B:626:LEU:C	1:B:626:LEU:HD23	2.39	0.47
1:A:64:HIS:O	1:A:66:PHE:N	2.48	0.47
1:A:434:SER:HA	1:A:436:ALA:N	2.30	0.47
1:B:298:SER:OG	1:B:374:VAL:HA	2.14	0.47
1:A:413:ASN:OD1	1:A:415:ASP:HB2	2.15	0.47
1:B:479:VAL:HA	1:B:633:ILE:HD13	1.96	0.47
1:A:535:GLY:C	1:A:537:GLY:H	2.23	0.47
1:B:223:TYR:HB3	1:B:226:VAL:HG13	1.97	0.46
1:B:7:LEU:CD2	1:B:181:ILE:HD11	2.45	0.46
1:B:226:VAL:HG22	1:B:229:PRO:CD	2.46	0.46
1:B:434:SER:HA	1:B:436:ALA:N	2.31	0.46
1:A:303:GLY:HA3	1:A:381:VAL:HG12	1.97	0.46
1:A:475:CYS:SG	1:A:638:MET:HG3	2.56	0.46
1:B:25:SER:O	1:B:26:PRO:C	2.58	0.46
1:B:401:PRO:HA	1:B:423:ARG:HH12	1.80	0.46
1:B:632:ARG:O	1:B:633:ILE:C	2.58	0.46
1:B:68:ALA:HB2	1:B:260:ALA:HA	1.98	0.45
1:A:98:LEU:CD1	3:A:1722:T1G:HACB	2.46	0.45
1:A:274:GLU:CD	1:A:657:ARG:HH22	2.24	0.45
1:A:372:SER:HA	1:A:399:CYS:HA	1.98	0.45
1:A:411:ALA:HB1	1:A:476:TYR:HE1	1.80	0.45
1:B:401:PRO:HA	1:B:423:ARG:NH1	2.32	0.45
1:B:63:ILE:HB	1:B:272:PHE:CZ	2.51	0.45
1:A:615:LYS:HE2	5:A:2036:HOH:O	2.16	0.45
3:B:1721:T1G:H3'	3:B:1721:T1G:PCB	2.57	0.45
1:A:25:SER:O	1:A:26:PRO:C	2.57	0.45
1:A:135:THR:HB	1:A:251:GLU:OE2	2.17	0.45
1:B:63:ILE:CD1	1:B:272:PHE:HE1	2.26	0.45
1:A:11:LEU:HD22	1:A:47:ALA:HB3	1.99	0.45
1:A:441:LEU:HD12	1:A:652:GLY:HA3	1.98	0.45
1:B:57:PHE:HA	5:B:2006:HOH:O	2.17	0.44
1:B:28:VAL:O	1:B:32:VAL:HG23	2.18	0.44
1:A:270:ALA:O	1:A:274:GLU:HG3	2.18	0.44
1:B:212:PHE:O	1:B:216:ILE:HG12	2.18	0.44
1:B:307:MET:SD	1:B:434:SER:HB3	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLU:HB3	1:B:332:LEU:HD12	2.00	0.44
1:B:292:SER:O	1:B:453:THR:HG23	2.17	0.44
1:B:595:LEU:HG	1:B:599:LEU:HD22	1.99	0.44
1:A:7:LEU:HD21	1:A:181:ILE:HD11	2.00	0.44
1:B:11:LEU:HD22	1:B:47:ALA:HB3	2.00	0.43
1:B:163:LEU:HB2	1:B:171:VAL:HG23	2.00	0.43
1:B:367:SER:C	1:B:369:LYS:H	2.25	0.43
1:B:427:VAL:O	1:B:450:SER:OG	2.35	0.43
1:B:433:PHE:O	1:B:439:MET:HB2	2.18	0.43
1:A:682:TYR:CE2	1:A:692:GLU:HG3	2.54	0.43
1:A:368:THR:HG23	5:A:2030:HOH:O	2.18	0.43
1:A:529:GLY:HA2	1:A:532:ILE:HD12	2.01	0.43
1:B:483:MET:HE3	1:B:630:ALA:HB2	2.01	0.43
1:B:25:SER:H	1:B:28:VAL:HB	1.84	0.43
1:B:402:GLY:N	5:B:2030:HOH:O	2.21	0.43
1:B:569:ARG:NH1	1:B:576:LYS:HE2	2.34	0.43
3:B:1721:T1G:HAX	3:B:1721:T1G:N7	2.34	0.43
1:A:63:ILE:HD13	1:A:63:ILE:HA	1.89	0.43
1:B:5:LEU:HB3	1:B:13:MET:HB3	2.01	0.42
1:A:113:ALA:HB3	1:A:168:LEU:HD13	2.01	0.42
1:B:56:ASN:HA	1:B:94:GLN:O	2.19	0.42
1:B:129:LEU:C	1:B:129:LEU:CD1	2.92	0.42
1:B:365:SER:HB2	1:B:370:GLU:OE2	2.20	0.42
1:A:582:ASP:OD1	1:A:586:GLY:HA3	2.20	0.42
1:B:14:ILE:HB	1:B:50:ILE:HG12	2.01	0.42
1:B:401:PRO:HA	5:B:2030:HOH:O	2.20	0.42
1:B:565:CYS:C	1:B:567:ALA:N	2.78	0.42
1:B:406:CYS:HA	1:B:428:ILE:O	2.20	0.42
1:A:597:THR:HG22	1:B:382:PHE:CZ	2.49	0.41
1:B:559:PRO:HG2	1:B:563:MET:HE3	2.02	0.41
1:B:629:GLU:O	1:B:633:ILE:HG13	2.19	0.41
1:B:486:PRO:CA	1:B:489[A]:ASN:ND2	2.69	0.41
1:B:527:ASP:OD2	1:B:573:LYS:NZ	2.50	0.41
1:B:7:LEU:HD13	1:B:13:MET:HB2	2.02	0.41
1:A:569:ARG:NH1	1:A:576:LYS:HE2	2.34	0.41
1:A:156:TYR:OH	3:A:1722:T1G:OAG	2.37	0.41
3:A:1722:T1G:OAG	3:A:1722:T1G:CAC	2.69	0.41
1:B:283:PRO:C	1:B:285:GLY:H	2.29	0.41
1:A:565:CYS:C	1:A:567:ALA:N	2.78	0.41
1:B:701:VAL:HG13	5:B:2047:HOH:O	2.21	0.41
1:A:66:PHE:HE2	1:A:128:ILE:HD13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:ARG:HD3	1:B:610:GLN:HG2	2.02	0.41
1:A:479:VAL:HG22	1:A:633:ILE:HG21	2.02	0.41
1:B:294:GLN:HG3	1:B:453:THR:CG2	2.50	0.41
1:B:434:SER:HA	1:B:435:PRO:C	2.46	0.41
1:B:68:ALA:CB	1:B:260:ALA:HA	2.51	0.41
1:B:359:LYS:HA	1:B:360:PRO:HD3	1.86	0.41
1:B:381:VAL:HA	2:B:1719:NAD:H52A	2.03	0.41
1:B:408:ASN:O	2:B:1719:NAD:H1D	2.21	0.41
1:A:433:PHE:CE1	1:A:441:LEU:HD13	2.56	0.40
1:A:279:LYS:N	1:A:279:LYS:HD3	2.35	0.40
1:B:129:LEU:HD12	1:B:129:LEU:O	2.21	0.40
1:A:298:SER:HB2	1:A:321:SER:HB2	2.03	0.40
1:A:490:GLN:O	1:A:494:LEU:HG	2.21	0.40
1:A:544:PRO:HA	1:A:545:PRO:HD3	1.99	0.40
1:B:283:PRO:HA	1:B:718:HIS:CE1	2.56	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	721/742 (97%)	671 (93%)	44 (6%)	6 (1%)	16	44
1	B	718/742 (97%)	667 (93%)	46 (6%)	5 (1%)	18	48
All	All	1439/1484 (97%)	1338 (93%)	90 (6%)	11 (1%)	16	44

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLY
1	A	284	SER
1	B	284	SER

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Mol	Chain	Res	Type
1	A	540	GLY
1	A	-1	SER
1	A	536	GLN
1	B	356	ALA
1	B	536	GLN
1	A	566	GLU
1	B	63	ILE
1	B	544	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	592/609 (97%)	539 (91%)	53 (9%)	9	28
1	B	591/609 (97%)	537 (91%)	54 (9%)	9	28
All	All	1183/1218 (97%)	1076 (91%)	107 (9%)	9	28

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	30	ARG
1	A	37	GLN
1	A	46	LYS
1	A	63	ILE
1	A	67	SER
1	A	73	LEU
1	A	86	GLN
1	A	96	VAL
1	A	125	THR
1	A	135	THR
1	A	144	VAL
1	A	157	LEU
1	A	165	LEU
1	A	172	VAL

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Mol	Chain	Res	Type
1	A	204	SER
1	A	219	VAL
1	A	226	VAL
1	A	234	ARG
1	A	245	GLU
1	A	249	LYS
1	A	258	LEU
1	A	299	VAL
1	A	306	THR
1	A	321	SER
1	A	330	LYS
1	A	333	ASP
1	A	340	THR
1	A	352	GLN
1	A	359	LYS
1	A	362	LEU
1	A	371	LEU
1	A	373	THR
1	A	390	LYS
1	A	398	LEU
1	A	407	THR
1	A	421	THR
1	A	425	GLN
1	A	441	LEU
1	A	445	ILE
1	A	463	LYS
1	A	508	LEU
1	A	523	LEU
1	A	528	VAL
1	A	549	VAL
1	A	572	GLN
1	A	585	LEU
1	A	609	GLU
1	A	610	GLN
1	A	626	LEU
1	A	675	LEU
1	A	676	GLU
1	A	720	SER
1	B	0	HIS
1	B	30	ARG
1	B	37	GLN
1	B	73	LEU

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Mol	Chain	Res	Type
1	B	86	GLN
1	B	90	LEU
1	B	96	VAL
1	B	125	THR
1	B	135	THR
1	B	144	VAL
1	B	157	LEU
1	B	161	GLU
1	B	163	LEU
1	B	165	LEU
1	B	203	PRO
1	B	204	SER
1	B	219	VAL
1	B	226	VAL
1	B	245	GLU
1	B	258	LEU
1	B	282	THR
1	B	287	SER
1	B	299	VAL
1	B	306	THR
1	B	321	SER
1	B	330	LYS
1	B	340	THR
1	B	351	HIS
1	B	352	GLN
1	B	359	LYS
1	B	362	LEU
1	B	371	LEU
1	B	373	THR
1	B	398	LEU
1	B	407	THR
1	B	421	THR
1	B	425	GLN
1	B	426	LEU
1	B	445	ILE
1	B	463	LYS
1	B	464	LYS
1	B	508	LEU
1	B	523	LEU
1	B	528	VAL
1	B	543	LEU
1	B	572	GLN

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Mol	Chain	Res	Type
1	B	585	LEU
1	B	596	SER
1	B	599	LEU
1	B	609	GLU
1	B	610	GLN
1	B	626	LEU
1	B	676	GLU
1	B	695	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	331	GLN
1	A	425	GLN
1	A	572	GLN
1	B	86	GLN
1	B	278	ASN
1	B	331	GLN
1	B	425	GLN
1	B	572	GLN
1	B	679	GLN
1	B	718	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](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	1723	-	4,4,4	0.36	0	6,6,6	0.37	0
3	T1G	B	1721	-	54,57,57	1.72	10 (18%)	75,85,85	2.31	21 (28%)
3	T1G	A	1722	-	54,57,57	1.54	7 (12%)	75,85,85	2.49	24 (32%)
2	NAD	B	1719	-	46,48,48	1.81	7 (15%)	64,73,73	1.66	8 (12%)
4	SO4	B	1722	-	4,4,4	0.21	0	6,6,6	0.42	0
4	SO4	B	1720	-	4,4,4	0.24	0	6,6,6	0.22	0
2	NAD	A	1721	-	46,48,48	2.00	8 (17%)	64,73,73	1.65	11 (17%)

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	T1G	A	1722	-	-	23/59/75/75	0/3/3/3
2	NAD	B	1719	-	-	15/30/62/62	0/5/5/5
3	T1G	B	1721	-	-	26/59/75/75	0/3/3/3
2	NAD	A	1721	-	-	8/30/62/62	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1721	NAD	O7N-C7N	9.50	1.41	1.24
2	B	1719	NAD	O7N-C7N	9.00	1.40	1.24
3	B	1721	T1G	PCB-OBJ	5.59	1.65	1.59
3	A	1722	T1G	PCA-OAI	4.63	1.64	1.50
3	A	1722	T1G	PCB-OAJ	4.18	1.65	1.50
2	A	1721	NAD	PA-O3	4.12	1.63	1.59
3	B	1721	T1G	PCB-OAJ	4.10	1.65	1.50
3	B	1721	T1G	PCA-OAI	4.06	1.63	1.50
3	B	1721	T1G	PCC-OAK	4.05	1.64	1.50
3	A	1722	T1G	PCC-OAK	3.92	1.64	1.50
2	A	1721	NAD	C2N-N1N	3.69	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1721	NAD	C2A-N3A	3.57	1.40	1.33
3	B	1721	T1G	PCA-O3'	3.50	1.65	1.59
2	A	1721	NAD	C2A-N1A	3.37	1.39	1.33
3	A	1722	T1G	PCB-OBJ	3.33	1.63	1.59
3	B	1721	T1G	PCC-OBJ	3.26	1.63	1.59
2	B	1719	NAD	PN-O3	3.06	1.62	1.59
2	B	1719	NAD	PA-O3	3.02	1.62	1.59
3	A	1722	T1G	C5-N7	-2.93	1.33	1.39
3	B	1721	T1G	C5-N7	-2.84	1.33	1.39
2	B	1719	NAD	C2A-N1A	2.76	1.38	1.33
3	B	1721	T1G	PCA-OAO	2.61	1.64	1.54
2	B	1719	NAD	C2A-N3A	2.50	1.38	1.33
3	A	1722	T1G	C8-N9	-2.50	1.33	1.37
2	A	1721	NAD	C8A-N7A	2.47	1.36	1.31
2	A	1721	NAD	C5A-N7A	-2.37	1.34	1.39
3	B	1721	T1G	C4-N9	-2.34	1.32	1.37
2	B	1719	NAD	C2N-N1N	2.28	1.37	1.35
3	B	1721	T1G	OAH-CBN	2.17	1.23	1.20
3	A	1722	T1G	PCA-OAO	2.16	1.62	1.54
2	B	1719	NAD	C8A-N7A	2.15	1.35	1.31
2	A	1721	NAD	PN-O3	2.11	1.61	1.59

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1722	T1G	OAH-CBN-SBK	-8.24	112.71	123.80
3	A	1722	T1G	O5'-PCB-OAJ	-7.37	79.72	108.94
3	B	1721	T1G	O5'-PCB-OAJ	-6.96	81.36	108.94
2	B	1719	NAD	N3A-C2A-N1A	-6.26	119.10	128.58
3	B	1721	T1G	OAH-CBN-SBK	-6.24	115.40	123.80
3	A	1722	T1G	C5-C4-N3	-6.01	118.44	126.72
2	A	1721	NAD	N3A-C2A-N1A	-5.66	120.02	128.58
3	A	1722	T1G	OAQ-PCB-OBJ	5.56	122.31	107.27
3	A	1722	T1G	N3-C2-N1	-5.48	120.29	128.58
3	B	1721	T1G	OAQ-PCB-O5'	-5.40	83.08	107.57
3	B	1721	T1G	OAQ-PCB-OBJ	5.39	121.85	107.27
3	A	1722	T1G	OAQ-PCB-O5'	-5.36	83.26	107.57
3	B	1721	T1G	C5-C4-N3	-5.36	119.34	126.72
2	A	1721	NAD	C5A-C4A-N3A	-5.18	119.59	126.72
3	B	1721	T1G	N3-C2-N1	-4.61	121.61	128.58
2	B	1719	NAD	C5A-C4A-N3A	-4.54	120.47	126.72
3	A	1722	T1G	CAC-CBZ-CAZ	-4.52	100.77	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1722	T1G	N3-C4-N9	4.22	134.34	127.17
3	A	1722	T1G	C2-N3-C4	4.20	122.08	111.83
3	B	1721	T1G	CAV-CAX-CBL	-3.96	105.80	112.39
3	B	1721	T1G	C2-N3-C4	3.77	121.03	111.83
2	A	1721	NAD	C2A-N3A-C4A	3.76	121.03	111.83
3	B	1721	T1G	C2'-C1'-N9	-3.73	104.04	113.30
2	B	1719	NAD	C2A-N3A-C4A	3.66	120.77	111.83
2	B	1719	NAD	N9A-C8A-N7A	-3.65	108.76	113.94
3	A	1722	T1G	CAW-SBK-CBN	3.62	112.13	101.73
3	B	1721	T1G	O4'-C1'-N9	3.55	114.90	108.09
3	B	1721	T1G	N3-C4-N9	3.54	133.18	127.17
2	B	1719	NAD	C5A-C6A-N6A	-3.49	114.64	123.29
2	B	1719	NAD	N3A-C4A-N9A	3.41	132.96	127.17
3	B	1721	T1G	N9-C8-N7	-3.41	109.11	113.94
2	A	1721	NAD	N3A-C4A-N9A	3.25	132.69	127.17
2	B	1719	NAD	C5A-N7A-C8A	3.20	108.48	103.45
3	A	1722	T1G	N9-C8-N7	-3.17	109.43	113.94
3	B	1721	T1G	C4-C5-N7	-3.11	107.02	110.58
3	B	1721	T1G	CAC-CBZ-CAZ	-3.10	103.10	108.22
3	B	1721	T1G	OBG-CAZ-CBZ	3.09	115.52	110.55
3	B	1721	T1G	C5-N7-C8	3.04	108.23	103.45
3	A	1722	T1G	C5-N7-C8	2.98	108.13	103.45
3	A	1722	T1G	C4-C5-N7	-2.97	107.18	110.58
3	A	1722	T1G	CAA-CBR-CBS	2.91	115.77	112.72
3	B	1721	T1G	PCA-O3'-C3'	2.80	130.92	123.43
3	A	1722	T1G	CAC-CBZ-CBT	2.76	113.47	108.77
2	A	1721	NAD	N9A-C8A-N7A	-2.75	110.04	113.94
3	A	1722	T1G	OAR-PCC-OBJ	2.74	114.69	107.27
2	A	1721	NAD	C5A-N7A-C8A	2.71	107.71	103.45
2	A	1721	NAD	O4B-C1B-N9A	2.68	113.24	108.09
3	A	1722	T1G	CAB-CBS-CBR	-2.64	109.24	111.92
3	A	1722	T1G	O4'-C1'-C2'	-2.55	101.16	106.62
3	A	1722	T1G	CAD-CBZ-CAZ	2.43	112.23	108.22
3	B	1721	T1G	C4-N9-C8	2.31	108.16	105.74
3	A	1722	T1G	C4-N9-C8	2.20	108.05	105.74
3	A	1722	T1G	CAU-NBD-CBL	2.19	126.91	122.82
3	B	1721	T1G	OAR-PCC-OBJ	2.19	113.19	107.27
2	A	1721	NAD	O2N-PN-O1N	2.17	122.52	112.44
3	A	1722	T1G	OAF-CBL-NBD	2.13	127.20	123.03
2	A	1721	NAD	C5A-C6A-N6A	-2.09	118.11	123.29
2	B	1719	NAD	C3N-C7N-N7N	2.08	120.30	117.74
3	A	1722	T1G	OAP-PCA-OAO	2.08	115.58	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1721	NAD	C6A-C5A-C4A	2.03	119.95	117.18
3	B	1721	T1G	C5'-C4'-C3'	-2.02	107.65	114.38
2	A	1721	NAD	O3-PN-O1N	-2.02	104.63	110.70
3	B	1721	T1G	CAB-CBS-CBR	-2.02	109.87	111.92
3	A	1722	T1G	OBG-CAZ-CBZ	2.01	113.77	110.55

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1721	NAD	O4D-C1D-N1N-C2N
2	A	1721	NAD	O4D-C1D-N1N-C6N
2	A	1721	NAD	C2D-C1D-N1N-C2N
2	A	1721	NAD	C2D-C1D-N1N-C6N
2	B	1719	NAD	C5B-O5B-PA-O1A
2	B	1719	NAD	C5B-O5B-PA-O2A
2	B	1719	NAD	C5B-O5B-PA-O3
2	B	1719	NAD	PN-O3-PA-O5B
2	B	1719	NAD	C5D-O5D-PN-O3
2	B	1719	NAD	C5D-O5D-PN-O1N
2	B	1719	NAD	C5D-O5D-PN-O2N
2	B	1719	NAD	O4D-C1D-N1N-C2N
3	A	1722	T1G	C5'-O5'-PCB-OAQ
3	A	1722	T1G	C5'-O5'-PCB-OBJ
3	A	1722	T1G	NBE-CAV-CAX-CBL
3	A	1722	T1G	OAH-CBN-SBK-CAW
3	A	1722	T1G	CBS-CBN-SBK-CAW
3	A	1722	T1G	CAA-CBR-CBS-CAB
3	A	1722	T1G	OAL-CBR-CBS-CAB
3	A	1722	T1G	OAL-CBR-CBS-CBN
3	A	1722	T1G	OAM-CBT-CBZ-CAC
3	A	1722	T1G	OAM-CBT-CBZ-CAD
3	A	1722	T1G	OAM-CBT-CBZ-CAZ
3	A	1722	T1G	CBM-CBT-CBZ-CAC
3	A	1722	T1G	CBM-CBT-CBZ-CAD
3	A	1722	T1G	CBM-CBT-CBZ-CAZ
3	B	1721	T1G	C5'-O5'-PCB-OAQ
3	B	1721	T1G	C5'-O5'-PCB-OBJ
3	B	1721	T1G	CAU-CAW-SBK-CBN
3	B	1721	T1G	OBG-CAZ-CBZ-CAC
3	B	1721	T1G	OBG-CAZ-CBZ-CAD
3	B	1721	T1G	OBG-CAZ-CBZ-CBT

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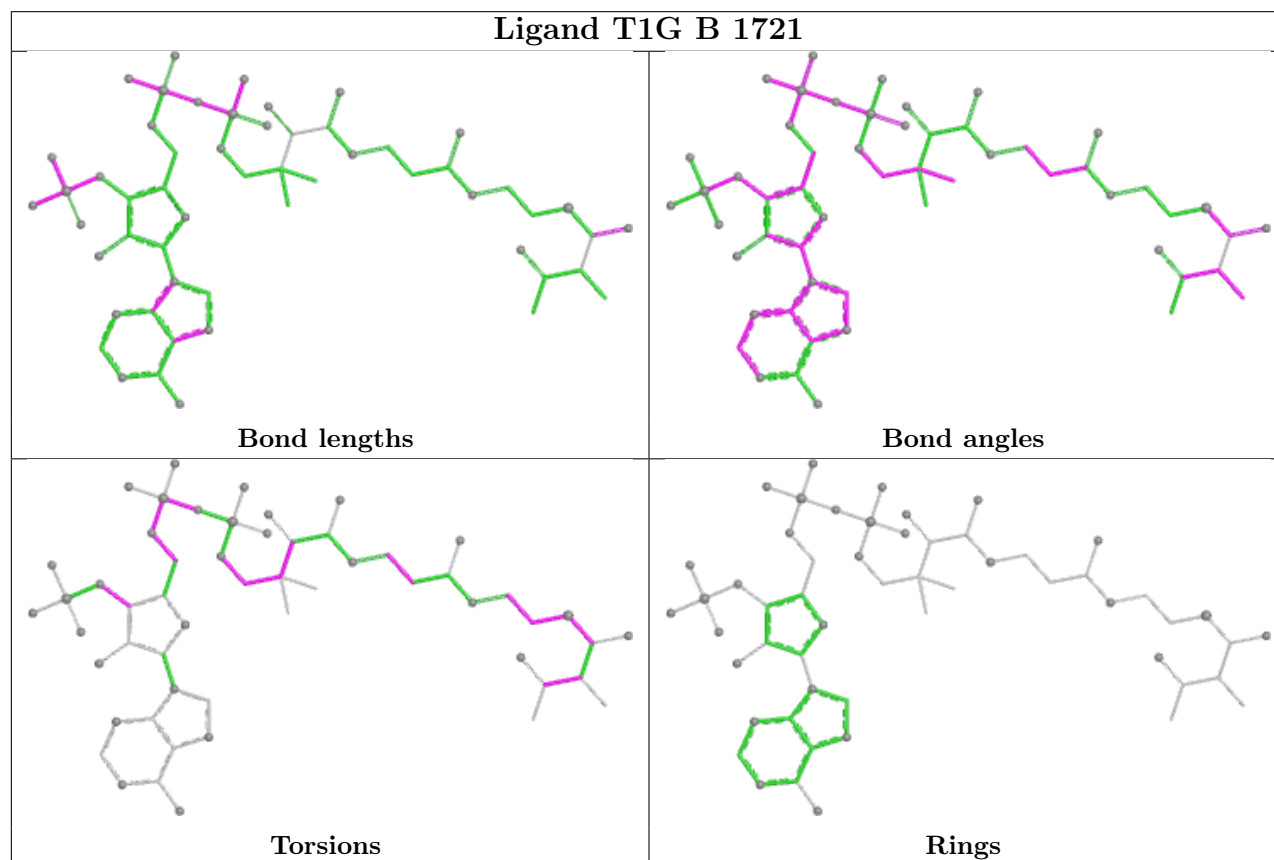
Mol	Chain	Res	Type	Atoms
3	B	1721	T1G	CBS-CBN-SBK-CAW
3	B	1721	T1G	CAA-CBR-CBS-CAB
3	B	1721	T1G	CAA-CBR-CBS-CBN
3	B	1721	T1G	OAL-CBR-CBS-CAB
3	B	1721	T1G	OAL-CBR-CBS-CBN
3	B	1721	T1G	OAM-CBT-CBZ-CAD
3	B	1721	T1G	OAM-CBT-CBZ-CAZ
3	B	1721	T1G	CBM-CBT-CBZ-CAC
3	B	1721	T1G	CBM-CBT-CBZ-CAD
3	B	1721	T1G	CBM-CBT-CBZ-CAZ
2	A	1721	NAD	C2N-C3N-C7N-O7N
2	A	1721	NAD	C2N-C3N-C7N-N7N
3	B	1721	T1G	C4'-C3'-O3'-PCA
2	B	1719	NAD	O4B-C4B-C5B-O5B
2	A	1721	NAD	C4N-C3N-C7N-N7N
3	B	1721	T1G	C2'-C3'-O3'-PCA
2	A	1721	NAD	C4N-C3N-C7N-O7N
2	B	1719	NAD	C3B-C4B-C5B-O5B
3	B	1721	T1G	NBD-CAU-CAW-SBK
3	B	1721	T1G	OAHCBN-SBK-CAW
3	B	1721	T1G	OAM-CBT-CBZ-CAC
3	A	1722	T1G	NBE-CBM-CBT-CBZ
2	B	1719	NAD	PA-O3-PN-O2N
3	A	1722	T1G	CAA-CBR-CBS-CBN
3	A	1722	T1G	C5'-O5'-PCB-OAJ
3	B	1721	T1G	C5'-O5'-PCB-OAJ
3	A	1722	T1G	SBK-CBN-CBS-CAB
3	B	1721	T1G	NBE-CAV-CAX-CBL
2	B	1719	NAD	PA-O3-PN-O1N
3	A	1722	T1G	OAG-CBM-CBT-CBZ
3	B	1721	T1G	C4'-C5'-O5'-PCB
2	B	1719	NAD	O4D-C4D-C5D-O5D
2	B	1719	NAD	O4D-C1D-N1N-C6N
3	A	1722	T1G	PCC-OBJ-PCB-OAQ
3	A	1722	T1G	PCB-OBJ-PCC-OAK
3	A	1722	T1G	PCB-OBJ-PCC-OAR
3	B	1721	T1G	PCC-OBJ-PCB-OAQ
3	A	1722	T1G	CBZ-CAZ-OBG-PCC
3	B	1721	T1G	CBZ-CAZ-OBG-PCC
2	B	1719	NAD	C3D-C4D-C5D-O5D

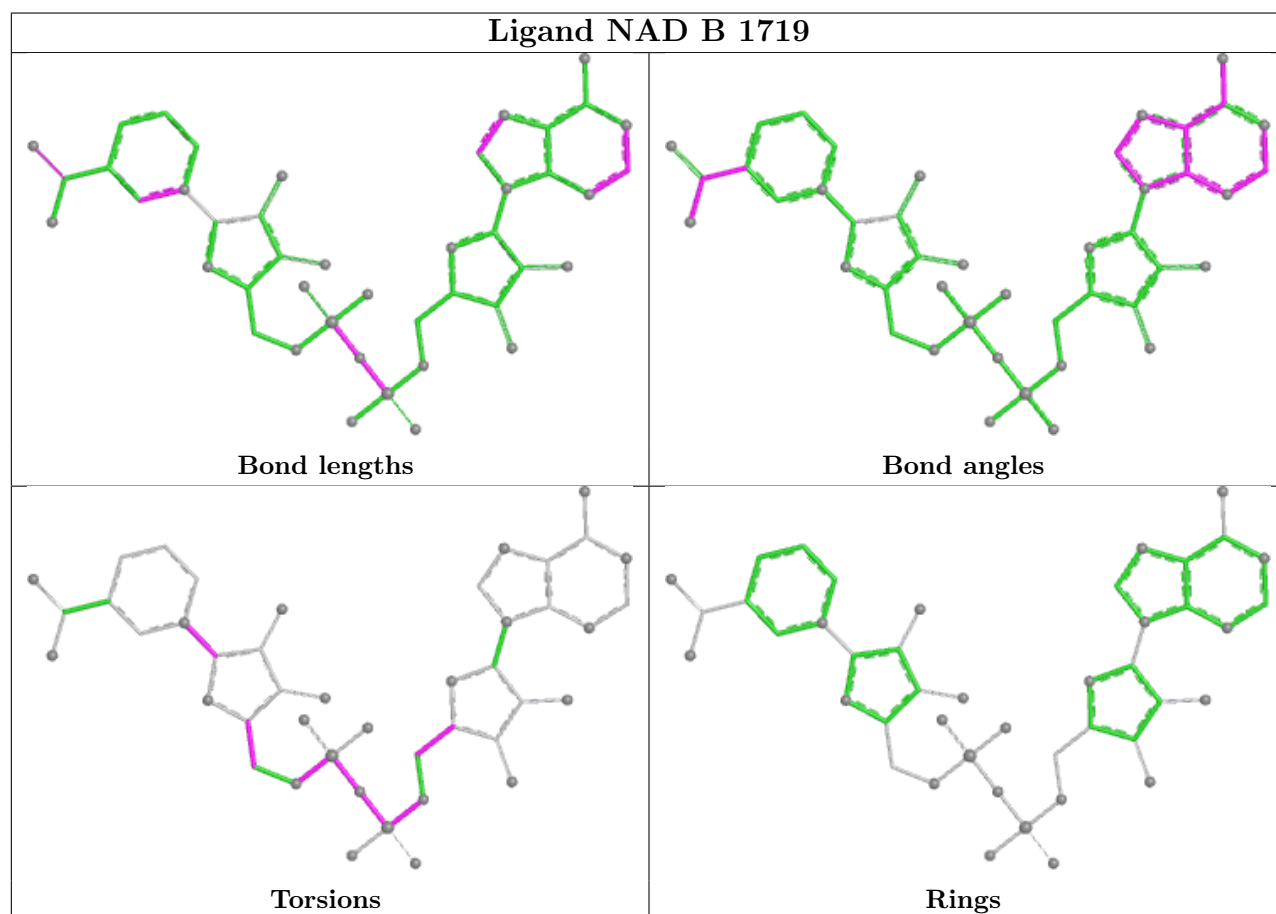
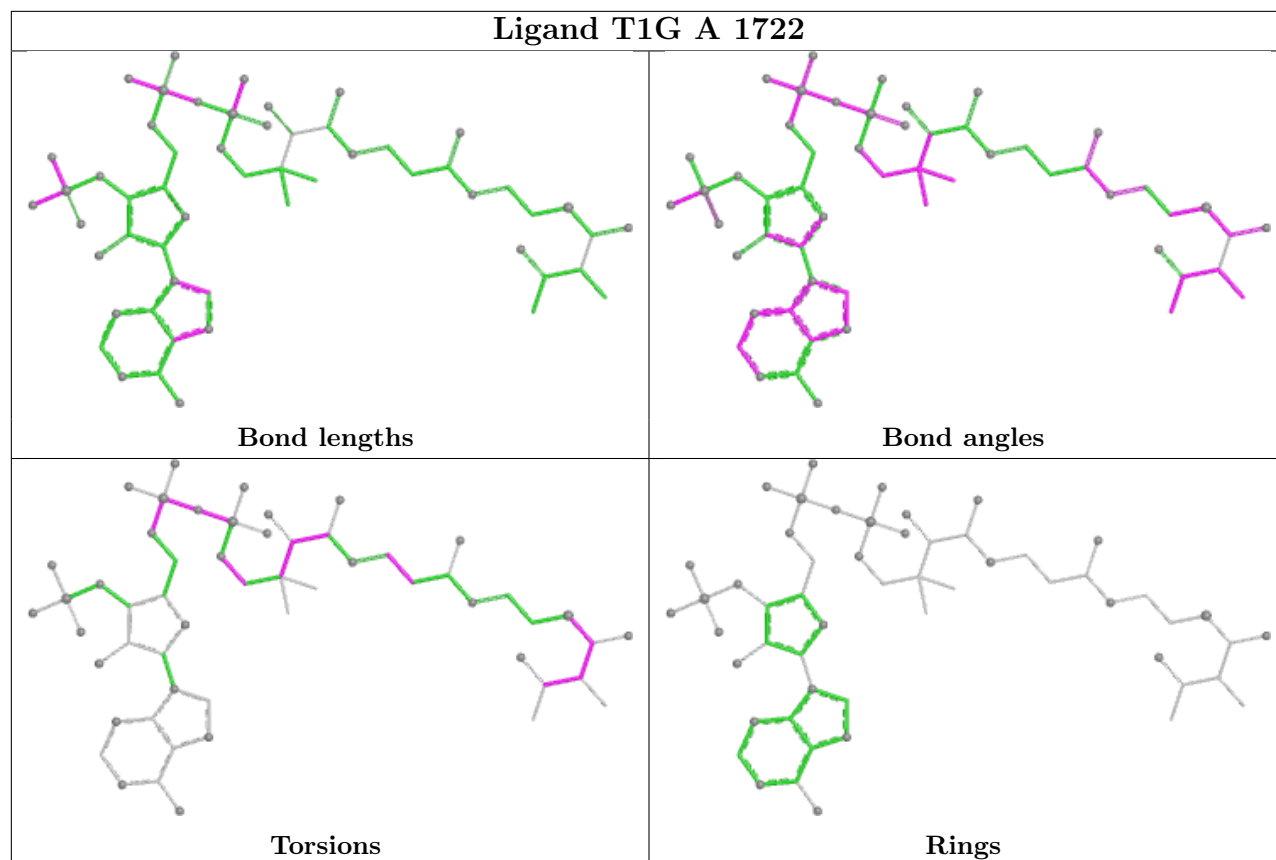
There are no ring outliers.

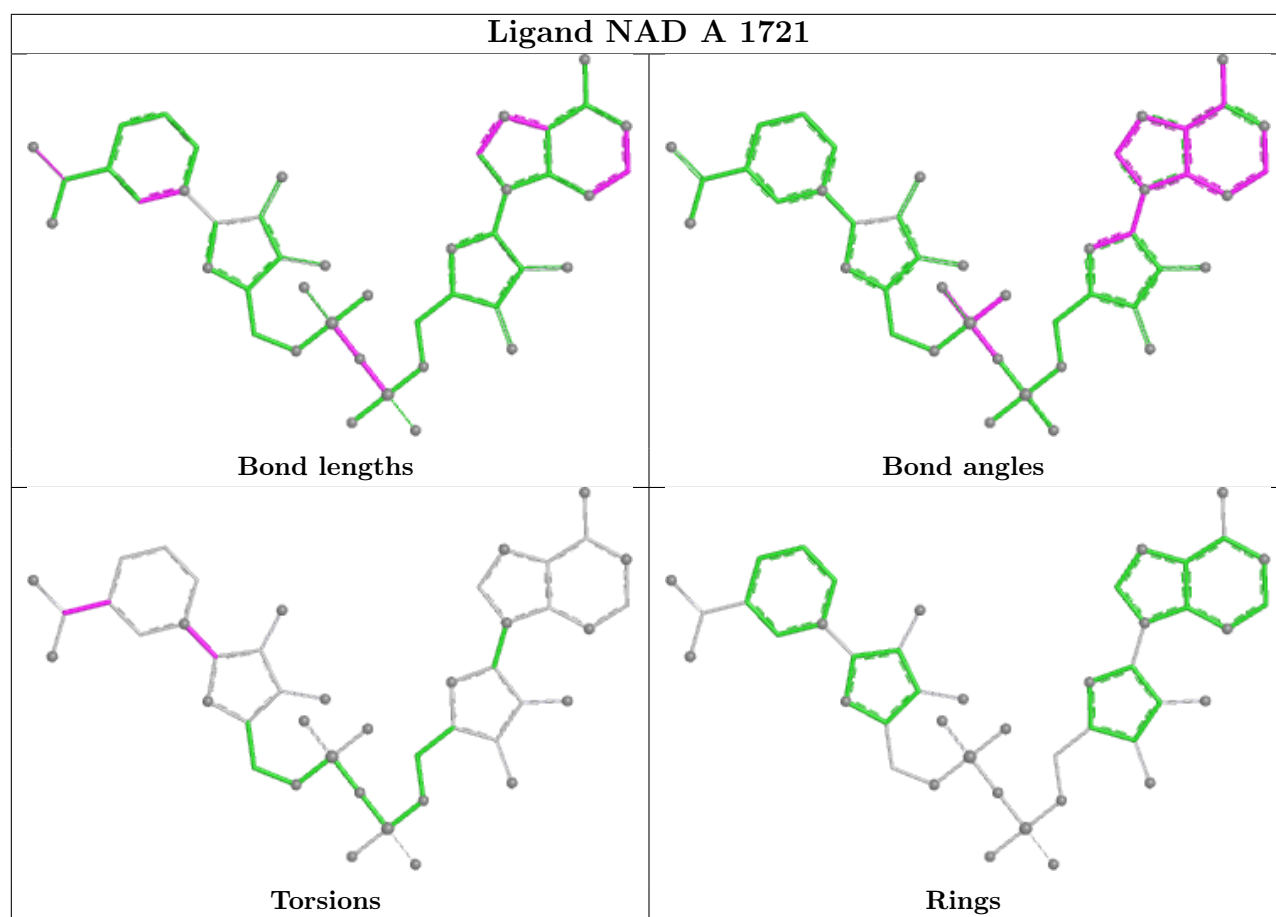
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1721	T1G	5	0
3	A	1722	T1G	5	0
2	B	1719	NAD	2	0
2	A	1721	NAD	2	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	723/742 (97%)	0.25	23 (3%)	50 41	16, 48, 92, 124	0
1	B	719/742 (96%)	0.20	18 (2%)	58 48	20, 49, 92, 124	1 (0%)
All	All	1442/1484 (97%)	0.22	41 (2%)	55 46	16, 49, 92, 124	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ALA	3.8
1	A	0	HIS	3.8
1	A	241	LYS	3.7
1	A	69	PHE	3.5
1	A	-2	GLY	3.5
1	B	713	SER	3.0
1	B	12	ALA	3.0
1	A	329	PRO	3.0
1	A	4	TYR	2.9
1	A	437	HIS	2.9
1	B	257	TYR	2.7
1	B	541	PRO	2.7
1	B	358	ALA	2.7
1	B	356	ALA	2.6
1	B	47	ALA	2.6
1	A	242	HIS	2.5
1	B	178	GLU	2.5
1	B	368	THR	2.5
1	A	6	ARG	2.5
1	B	43	HIS	2.5
1	A	324	ALA	2.4
1	A	536	GLN	2.4
1	A	718	HIS	2.4
1	A	5	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	41	SER	2.4
1	B	718	HIS	2.4
1	B	53	ALA	2.3
1	A	387	LEU	2.2
1	B	170	ALA	2.2
1	A	37	GLN	2.2
1	B	171	VAL	2.1
1	A	1	MET	2.1
1	A	364	PHE	2.1
1	B	351	HIS	2.1
1	B	176	PRO	2.1
1	B	63	ILE	2.1
1	A	351	HIS	2.1
1	A	2	ALA	2.1
1	A	348	SER	2.1
1	A	358	ALA	2.1
1	B	366	SER	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.

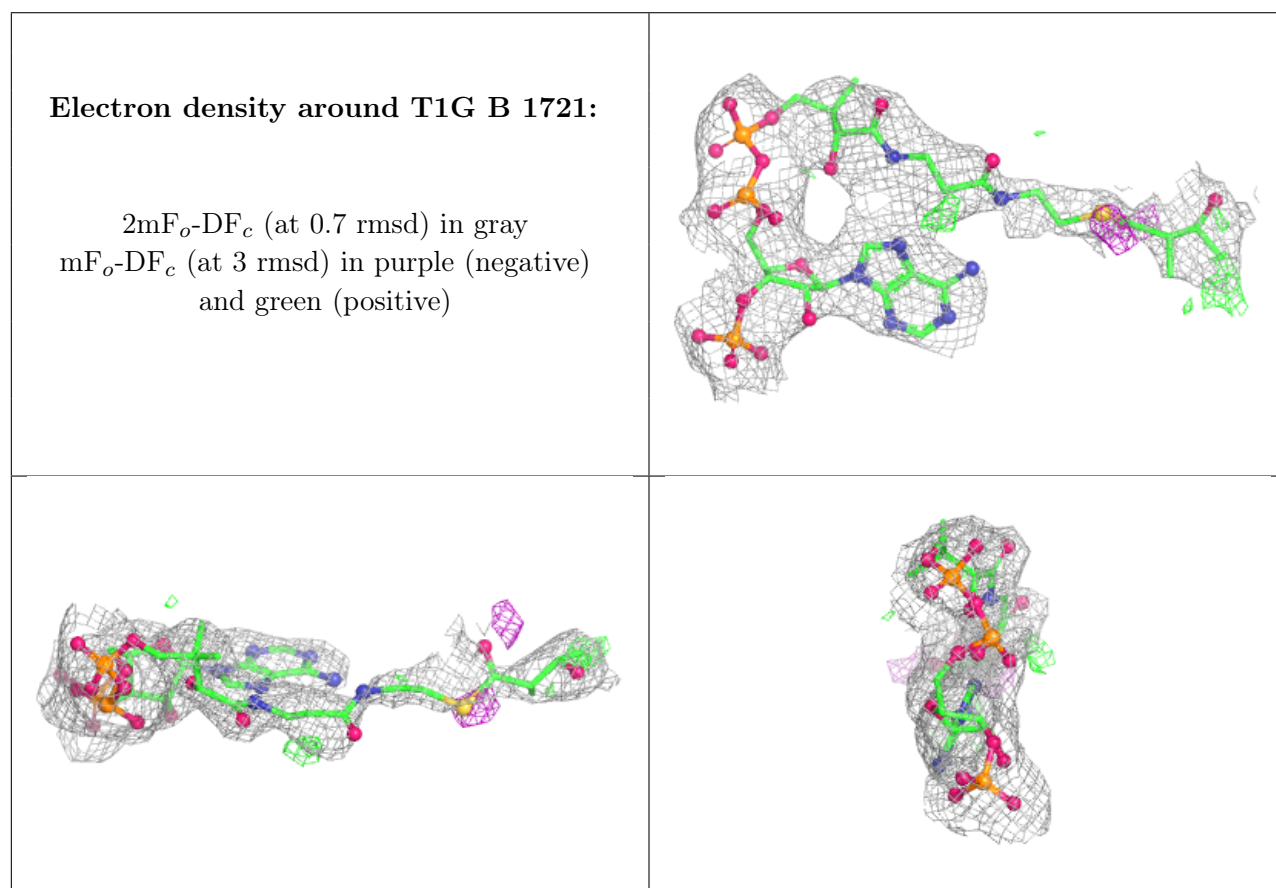
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	T1G	B	1721	55/55	0.82	0.15	70,95,100,102	0
4	SO4	B	1722	5/5	0.83	0.12	93,94,95,95	0
4	SO4	B	1720	5/5	0.85	0.13	82,83,84,84	0
3	T1G	A	1722	55/55	0.86	0.12	37,58,67,69	0
2	NAD	A	1721	44/44	0.86	0.12	77,80,82,83	0
2	NAD	B	1719	44/44	0.90	0.10	72,75,76,76	0

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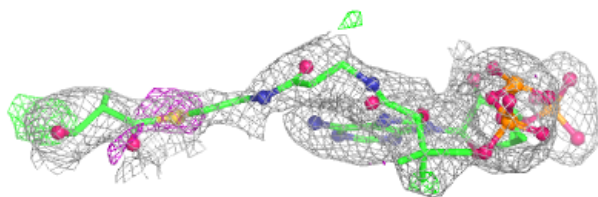
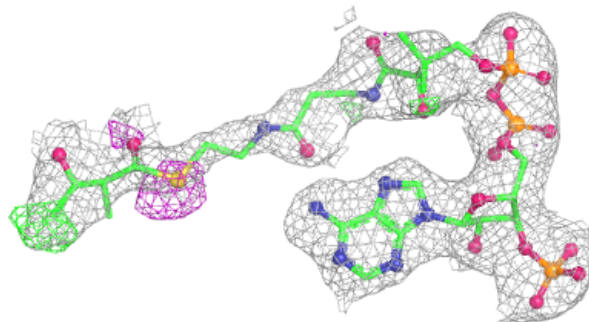
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1723	5/5	0.95	0.10	46,47,49,50	0

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

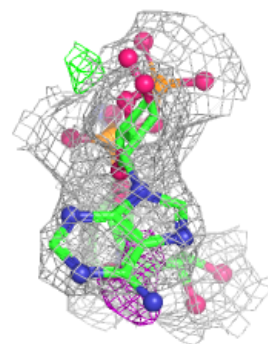
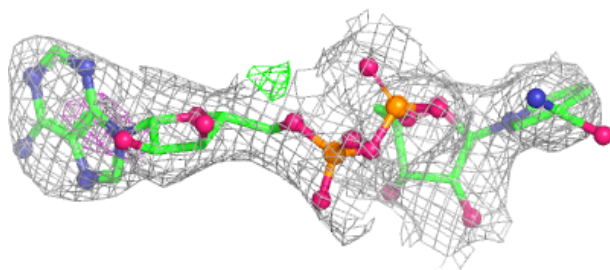
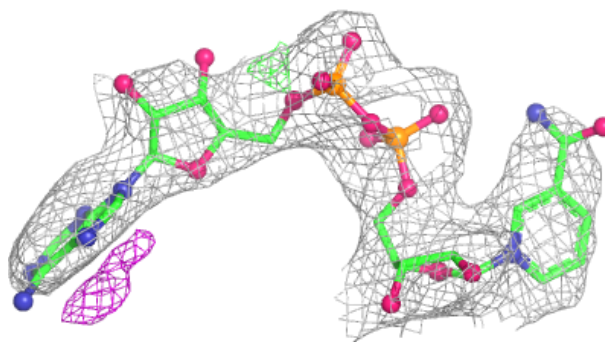


Electron density around T1G A 1722:

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

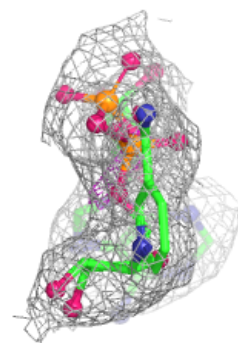
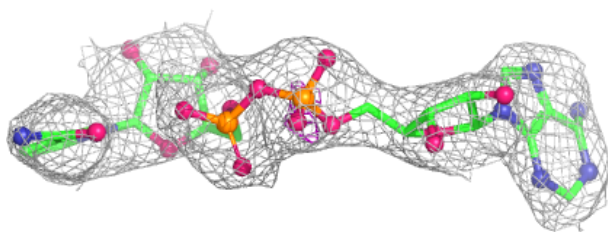
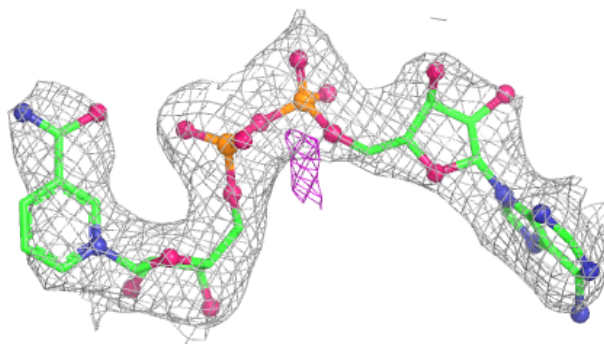
**Electron density around NAD A 1721:**

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



Electron density around NAD B 1719:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.