



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:02 AM UTC

PDB ID : 2X0N / pdb_00002x0n
Title : Structure of glycosomal glyceraldehyde-3-phosphate dehydrogenase from Trypanosoma brucei determined from Laue data
Authors : Vellieux, F.M.D.; Hajdu, J.; Hol, W.G.J.
Deposited on : 2009-12-16
Resolution : 3.20 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

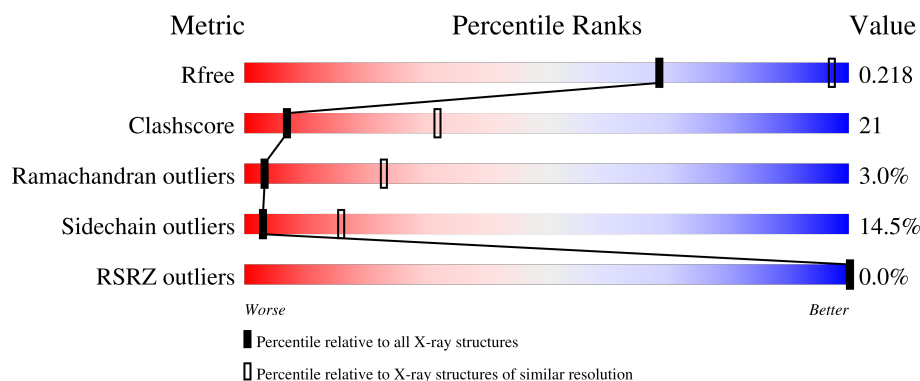
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	
1	B	359	
1	O	359	
1	P	359	
1	Q	359	

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Mol	Chain	Length	Quality of chain
1	R	359	62% 30% 8%

2 Entry composition [i](#)

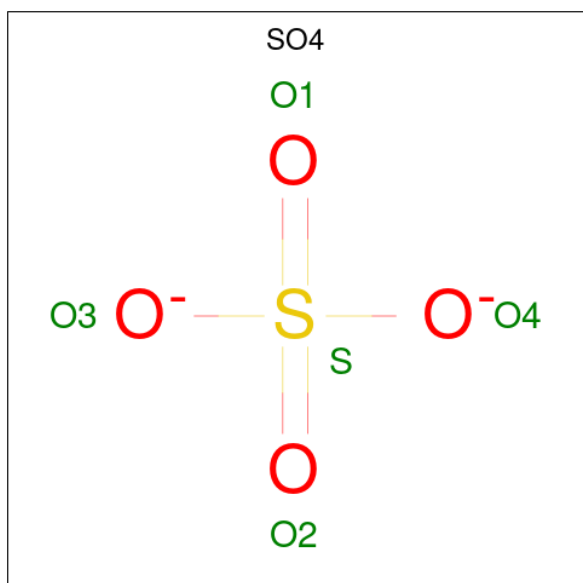
There are 3 unique types of molecules in this entry. The entry contains 16734 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

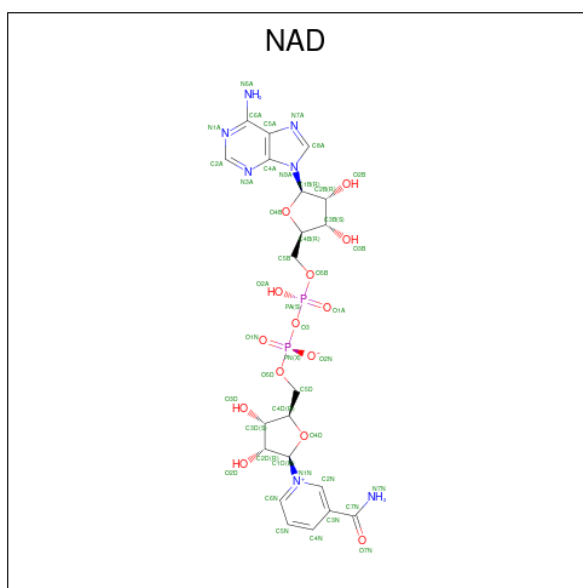
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			
1	B	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			
1	O	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			
1	P	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			
1	Q	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			
1	R	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	O	1	Total 5	O 4	S 1	0	0
2	O	1	Total 5	O 4	S 1	0	0
2	P	1	Total 5	O 4	S 1	0	0
2	P	1	Total 5	O 4	S 1	0	0
2	Q	1	Total 5	O 4	S 1	0	0
2	Q	1	Total 5	O 4	S 1	0	0
2	R	1	Total 5	O 4	S 1	0	0
2	R	1	Total 5	O 4	S 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).

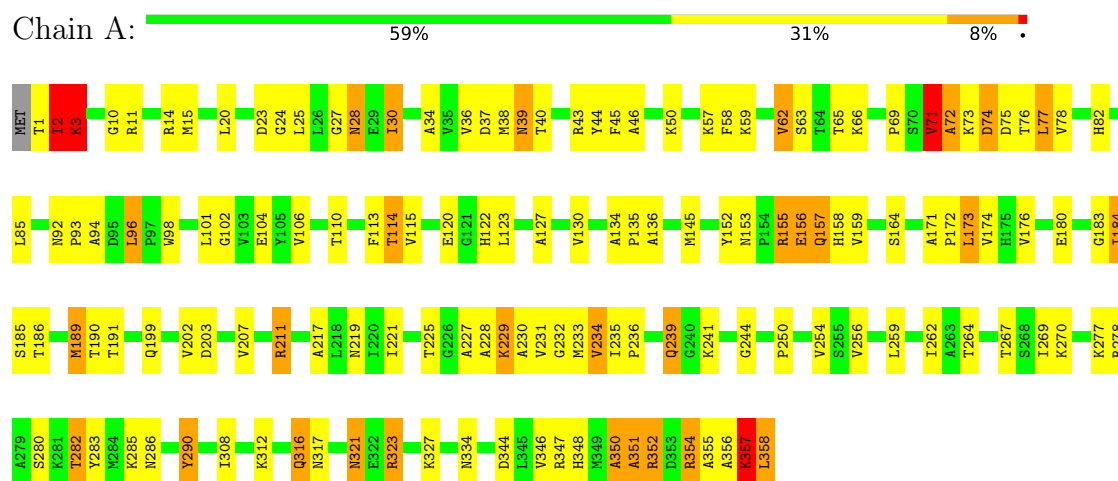


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

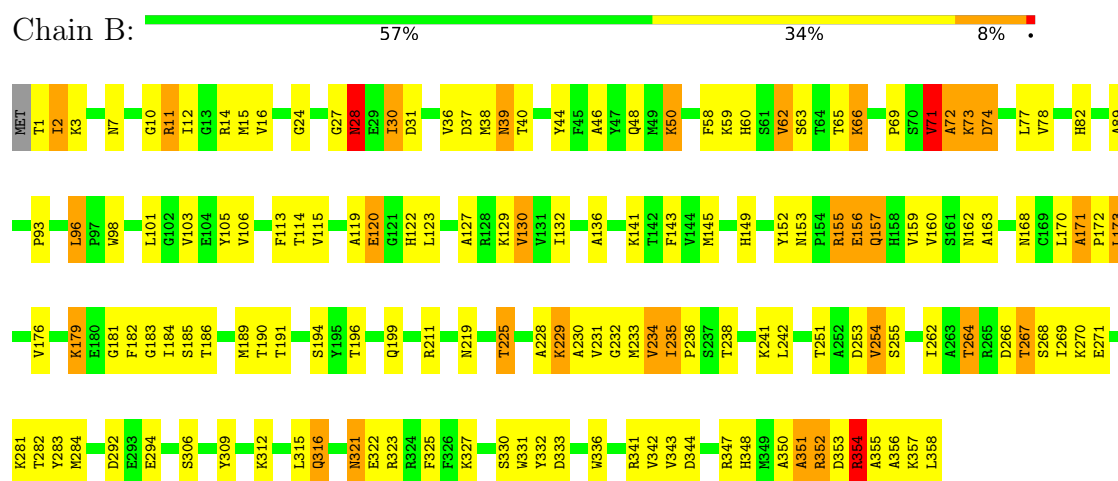
3 Residue-property plots

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

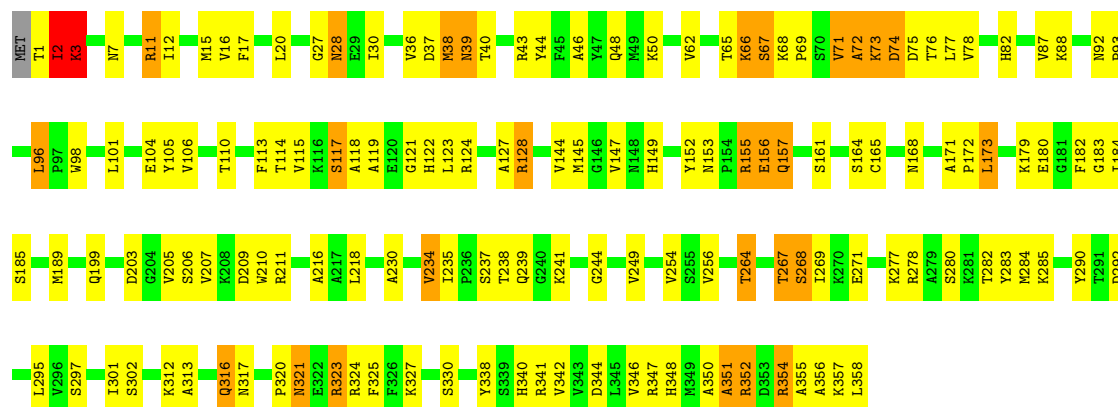


- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE, GLYCOSOMAL



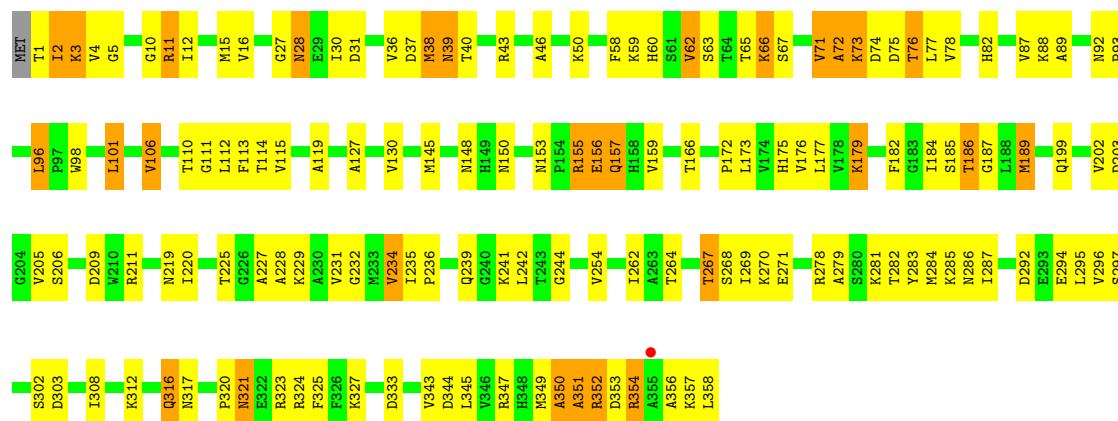
- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE, GLYCOSOMAL





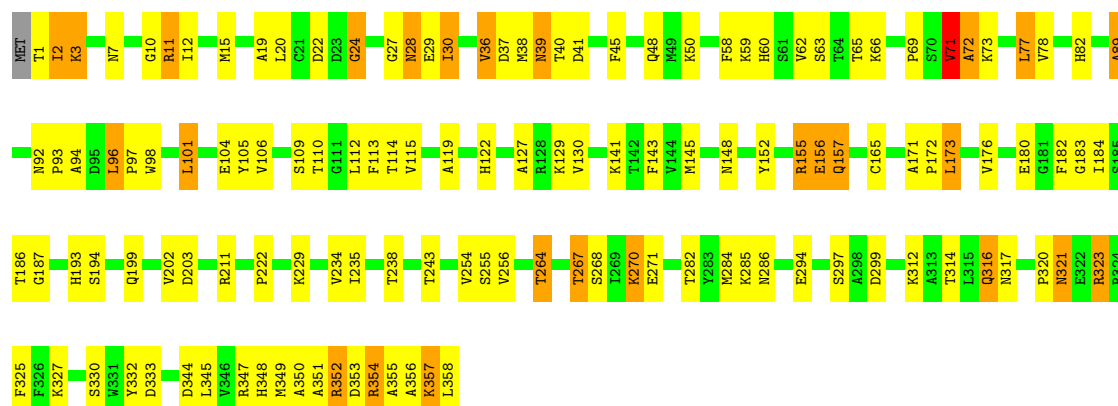
- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE, GLYCOSOMAL

Chain P: 58% 33% 8%



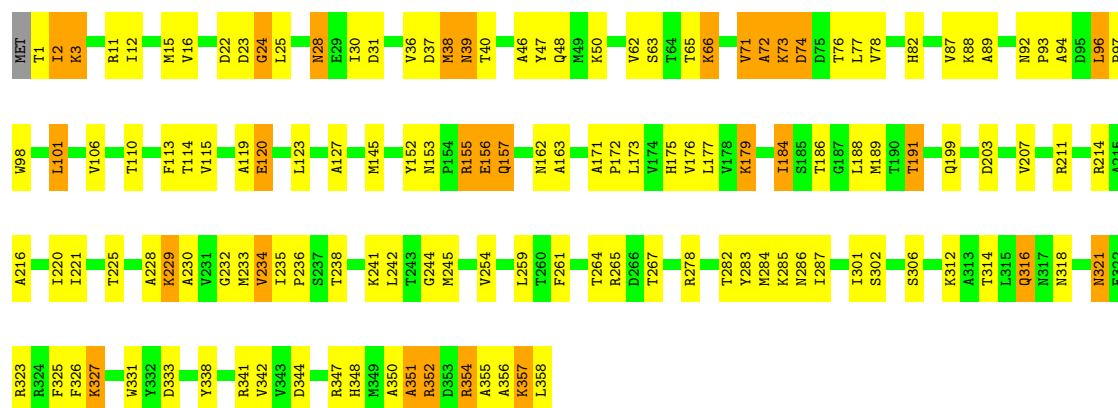
- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE, GLYCOSOMAL

Chain Q: 63% 30% 7%



- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE, GLYCOSOMAL

Chain R:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.52Å 256.27Å 114.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.40 – 3.20 7.40 – 3.20	Depositor EDS
% Data completeness (in resolution range)	57.3 (7.40-3.20) 52.4 (7.40-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 3.22Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.150 , 0.218 0.150 , 0.218	Depositor DCC
R_{free} test set	1798 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 91.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16734	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9661e-03.*

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: 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	0.58	0/2785	0.98	10/3770 (0.3%)
1	B	0.58	0/2785	1.01	10/3770 (0.3%)
1	O	0.61	0/2785	0.99	6/3770 (0.2%)
1	P	0.61	0/2785	0.98	3/3770 (0.1%)
1	Q	0.60	0/2785	0.98	4/3770 (0.1%)
1	R	0.58	0/2785	0.98	5/3770 (0.1%)
All	All	0.59	0/16710	0.99	38/22620 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	244	GLY	N-CA-C	7.01	120.98	110.75
1	B	219	ASN	N-CA-C	6.82	119.53	109.24
1	B	235	ILE	CA-C-N	6.62	126.56	119.28
1	B	235	ILE	C-N-CA	6.62	126.56	119.28
1	O	3	LYS	N-CA-C	6.46	120.12	108.17
1	Q	71	VAL	N-CA-C	6.40	117.31	111.81
1	R	155	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	A	221	ILE	N-CA-C	6.30	114.39	108.15
1	B	336	TRP	N-CA-C	6.27	117.80	110.97
1	R	155	ARG	CD-NE-CZ	-6.24	115.67	124.40
1	P	317	ASN	N-CA-C	6.05	120.39	111.87
1	A	180	GLU	N-CA-C	-6.04	105.89	113.20
1	A	44	TYR	N-CA-C	-5.98	104.84	111.36
1	B	171	ALA	CA-C-N	5.91	125.78	119.28
1	B	171	ALA	C-N-CA	5.91	125.78	119.28
1	R	244	GLY	N-CA-C	5.80	119.22	110.75
1	P	279	ALA	N-CA-C	-5.63	106.24	113.23
1	A	317	ASN	N-CA-C	5.58	119.90	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	180	GLU	N-CA-C	-5.46	106.47	113.02
1	R	184	ILE	CB-CA-C	-5.44	105.05	111.09
1	A	3	LYS	N-CA-C	5.40	117.27	108.63
1	B	71	VAL	N-CA-C	5.40	116.27	111.90
1	A	308	ILE	N-CA-C	5.38	115.28	106.72
1	B	196	THR	N-CA-C	5.36	116.80	109.18
1	P	308	ILE	N-CA-C	5.35	115.79	107.28
1	A	71	VAL	N-CA-C	5.30	118.26	112.96
1	A	219	ASN	N-CA-C	5.26	117.19	109.24
1	Q	256	VAL	N-CA-C	5.25	115.28	108.35
1	A	244	GLY	N-CA-C	5.24	118.23	110.42
1	O	283	TYR	N-CA-C	5.19	118.87	112.54
1	B	309	TYR	N-CA-C	5.19	116.71	108.67
1	A	221	ILE	CB-CA-C	-5.17	106.17	111.08
1	R	216	ALA	N-CA-C	5.14	116.97	111.36
1	O	216	ALA	N-CA-C	5.10	116.84	111.28
1	Q	187	GLY	N-CA-C	5.07	118.67	110.87
1	O	249	VAL	CA-C-N	5.04	126.13	119.84
1	O	249	VAL	C-N-CA	5.04	126.13	119.84
1	B	28	ASN	N-CA-C	-5.01	107.12	113.43

There are no chirality outliers.

There are no planarity outliers.

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	2735	0	2757	123	0
1	B	2735	0	2757	122	0
1	O	2735	0	2757	127	0
1	P	2735	0	2757	121	0
1	Q	2735	0	2757	119	0
1	R	2735	0	2757	116	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	O	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	10	0	0	1	0
2	Q	10	0	0	0	0
2	R	10	0	0	1	0
3	A	44	0	26	2	0
3	B	44	0	26	3	0
3	O	44	0	26	3	0
3	P	44	0	26	3	0
3	Q	44	0	26	6	0
3	R	44	0	26	3	0
All	All	16734	0	16698	701	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 21.

All (701) 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:155:ARG:HH11	1:B:155:ARG:HG2	1.01	1.12
1:Q:155:ARG:HG2	1:Q:155:ARG:HH11	1.10	1.11
1:A:155:ARG:HG2	1:A:155:ARG:HH11	1.12	1.09
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.10	1.07
1:O:155:ARG:HG2	1:O:155:ARG:HH11	1.15	1.05
1:P:155:ARG:HG2	1:P:155:ARG:HH11	1.20	1.04
1:A:347:ARG:NH2	1:A:358:LEU:HD23	1.75	1.01
1:A:156:GLU:OE1	1:A:156:GLU:HA	1.59	0.98
1:B:156:GLU:HA	1:B:156:GLU:OE1	1.64	0.98
1:A:357:LYS:HG2	1:A:358:LEU:N	1.78	0.96
1:O:347:ARG:NH2	1:O:358:LEU:HD22	1.81	0.95
1:A:347:ARG:HH21	1:A:358:LEU:HD23	1.29	0.95
1:B:46:ALA:O	1:B:50:LYS:HG3	1.65	0.95
1:O:128:ARG:CG	1:O:128:ARG:HH11	1.79	0.93
1:R:156:GLU:OE1	1:R:156:GLU:HA	1.67	0.92
1:A:46:ALA:O	1:A:50:LYS:HG3	1.71	0.90
1:Q:155:ARG:HG2	1:Q:155:ARG:NH1	1.83	0.90
1:Q:156:GLU:HA	1:Q:156:GLU:OE1	1.71	0.88
1:B:155:ARG:HG2	1:B:155:ARG:NH1	1.81	0.88
1:O:156:GLU:HA	1:O:156:GLU:OE1	1.72	0.87
1:O:347:ARG:HH21	1:O:358:LEU:HD22	1.39	0.87
1:P:156:GLU:OE1	1:P:156:GLU:HA	1.72	0.87
1:A:2:ILE:HG23	1:A:3:LYS:H	1.39	0.87
1:P:96:LEU:HD12	1:P:98:TRP:CZ2	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ARG:O	1:B:15:MET:HG2	1.74	0.86
1:P:2:ILE:HG23	1:P:3:LYS:H	1.38	0.86
1:O:155:ARG:HG2	1:O:155:ARG:NH1	1.86	0.86
1:O:155:ARG:HH11	1:O:155:ARG:CG	1.89	0.85
1:Q:2:ILE:HG23	1:Q:3:LYS:H	1.42	0.84
1:A:323:ARG:HG2	1:A:323:ARG:NH1	1.86	0.84
1:R:11:ARG:O	1:R:15:MET:HG2	1.77	0.84
1:B:347:ARG:HH21	1:B:358:LEU:HD22	1.43	0.83
1:A:155:ARG:HG2	1:A:155:ARG:NH1	1.88	0.83
1:R:347:ARG:HH21	1:R:358:LEU:HD13	1.44	0.82
1:P:65:THR:HG22	1:P:66:LYS:H	1.44	0.82
1:O:323:ARG:HG3	1:O:323:ARG:HH11	1.44	0.82
1:B:2:ILE:HG23	1:B:3:LYS:H	1.46	0.81
1:Q:352:ARG:C	1:Q:354:ARG:H	1.88	0.81
1:Q:155:ARG:HH11	1:Q:155:ARG:CG	1.92	0.81
1:A:321:ASN:N	1:A:321:ASN:HD22	1.81	0.79
1:O:323:ARG:HH11	1:O:323:ARG:CG	1.95	0.79
1:O:323:ARG:HG3	1:O:323:ARG:NH1	1.97	0.78
1:Q:145:MET:HE2	1:Q:344:ASP:HB3	1.67	0.77
1:P:11:ARG:O	1:P:15:MET:HG2	1.84	0.77
1:Q:11:ARG:O	1:Q:15:MET:HG2	1.85	0.77
1:B:155:ARG:HH11	1:B:155:ARG:CG	1.92	0.77
1:Q:165:CYS:HB3	3:Q:361:NAD:H4N	1.65	0.77
1:Q:347:ARG:NH2	1:Q:358:LEU:HD22	2.00	0.76
1:A:11:ARG:O	1:A:15:MET:HG2	1.84	0.76
1:B:228:ALA:HB1	1:B:242:LEU:HB3	1.66	0.76
1:A:155:ARG:HH11	1:A:155:ARG:CG	1.97	0.76
1:O:128:ARG:HH11	1:O:128:ARG:HG3	1.49	0.76
1:A:277:LYS:O	1:A:280:SER:HB2	1.86	0.76
1:P:65:THR:HG22	1:P:66:LYS:N	1.99	0.76
1:P:155:ARG:HH11	1:P:155:ARG:CG	1.96	0.76
1:B:65:THR:HG22	1:B:66:LYS:N	2.00	0.75
1:B:38:MET:O	1:B:39:ASN:HB3	1.85	0.75
1:Q:347:ARG:HH21	1:Q:358:LEU:HD22	1.50	0.74
1:A:312:LYS:O	1:A:316:GLN:HB2	1.87	0.74
1:A:352:ARG:C	1:A:354:ARG:H	1.95	0.74
1:O:11:ARG:NH1	1:R:203:ASP:HB2	2.03	0.74
1:O:2:ILE:HG23	1:O:3:LYS:H	1.50	0.74
1:Q:323:ARG:HH11	1:Q:323:ARG:CG	2.00	0.74
1:A:38:MET:O	1:A:39:ASN:HB3	1.87	0.74
1:O:11:ARG:HH12	1:R:203:ASP:HB2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:128:ARG:HH11	1:O:128:ARG:HG2	1.53	0.73
1:O:11:ARG:O	1:O:15:MET:HG2	1.88	0.73
1:R:65:THR:HG22	1:R:66:LYS:N	2.02	0.73
1:Q:11:ARG:HB2	3:Q:361:NAD:O2N	1.89	0.72
1:O:352:ARG:HG2	1:O:352:ARG:HH11	1.53	0.72
1:P:155:ARG:HG2	1:P:155:ARG:NH1	1.91	0.72
1:Q:2:ILE:HG23	1:Q:3:LYS:N	2.04	0.72
1:A:262:ILE:HD11	1:B:262:ILE:HD11	1.72	0.71
1:P:2:ILE:HG23	1:P:3:LYS:N	2.06	0.71
1:B:66:LYS:HD3	1:B:69:PRO:HA	1.73	0.71
1:P:345:LEU:O	1:P:349:MET:HG3	1.90	0.71
1:P:352:ARG:C	1:P:354:ARG:H	1.99	0.71
1:R:38:MET:O	1:R:39:ASN:HB3	1.90	0.70
1:Q:312:LYS:O	1:Q:316:GLN:HB2	1.91	0.70
1:O:38:MET:O	1:O:39:ASN:HB3	1.92	0.70
1:R:352:ARG:C	1:R:354:ARG:H	1.99	0.70
1:O:325:PHE:HE1	1:P:325:PHE:HE1	1.39	0.69
1:P:153:ASN:ND2	1:P:156:GLU:HG2	2.07	0.69
1:O:352:ARG:HG2	1:O:352:ARG:NH1	2.06	0.69
1:Q:1:THR:CG2	1:Q:30:ILE:HG23	2.23	0.69
1:B:7:ASN:HD22	1:B:122:HIS:HE1	1.39	0.69
1:O:93:PRO:HG3	1:O:113:PHE:CE1	2.28	0.69
1:P:38:MET:O	1:P:39:ASN:HB3	1.93	0.69
1:A:65:THR:HG22	1:A:66:LYS:N	2.08	0.68
1:P:352:ARG:NH1	1:P:352:ARG:HG2	2.08	0.68
1:A:230:ALA:O	1:A:233:MET:HB2	1.93	0.68
1:Q:65:THR:HG22	1:Q:66:LYS:N	2.08	0.68
1:A:323:ARG:HH11	1:A:323:ARG:CG	1.95	0.68
1:P:63:SER:HB3	1:P:78:VAL:HB	1.76	0.68
1:P:37:ASP:O	1:P:89:ALA:HB2	1.94	0.67
1:A:352:ARG:HG2	1:A:352:ARG:HH11	1.59	0.67
1:B:321:ASN:N	1:B:321:ASN:HD22	1.90	0.67
1:P:234:VAL:HG12	1:P:235:ILE:HG13	1.75	0.67
1:Q:323:ARG:HH11	1:Q:323:ARG:HG3	1.59	0.67
1:B:65:THR:HG22	1:B:66:LYS:H	1.58	0.67
1:R:321:ASN:N	1:R:321:ASN:HD22	1.91	0.67
1:R:338:TYR:O	1:R:342:VAL:HG23	1.94	0.67
1:R:2:ILE:HG23	1:R:3:LYS:H	1.58	0.67
1:A:352:ARG:HG2	1:A:352:ARG:NH1	2.10	0.67
1:R:65:THR:HG22	1:R:66:LYS:H	1.59	0.67
1:Q:2:ILE:CG2	1:Q:3:LYS:H	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:HG12	1:A:235:ILE:HG13	1.76	0.67
1:P:203:ASP:HB2	1:Q:11:ARG:HH12	1.60	0.67
1:B:354:ARG:NH1	1:B:354:ARG:HB2	2.08	0.66
1:R:46:ALA:O	1:R:50:LYS:HG3	1.96	0.66
1:P:352:ARG:HG2	1:P:352:ARG:HH11	1.61	0.66
1:R:352:ARG:NH1	1:R:352:ARG:HG2	2.10	0.66
1:B:27:GLY:HA3	1:B:82:HIS:NE2	2.11	0.65
1:R:93:PRO:HG3	1:R:113:PHE:CE1	2.31	0.65
1:O:352:ARG:C	1:O:354:ARG:H	2.04	0.65
1:Q:350:ALA:O	1:Q:355:ALA:HB3	1.96	0.65
1:R:1:THR:HG22	1:R:30:ILE:HG12	1.79	0.65
1:P:71:VAL:O	1:P:72:ALA:HB3	1.97	0.65
1:B:12:ILE:O	1:B:16:VAL:HG23	1.97	0.64
1:O:171:ALA:HB3	1:O:172:PRO:HD3	1.80	0.64
1:Q:352:ARG:NH1	1:Q:352:ARG:HG2	2.13	0.64
1:B:145:MET:HE2	1:B:344:ASP:HB3	1.79	0.64
1:O:321:ASN:HD22	1:O:321:ASN:N	1.96	0.64
1:A:71:VAL:O	1:A:72:ALA:HB3	1.96	0.64
1:B:96:LEU:HD12	1:B:98:TRP:CZ2	2.32	0.64
1:B:171:ALA:HB3	1:B:172:PRO:HD3	1.79	0.64
1:O:128:ARG:HG2	1:O:128:ARG:NH1	2.11	0.64
1:Q:122:HIS:O	1:Q:127:ALA:HB3	1.98	0.64
1:A:171:ALA:HB3	1:A:172:PRO:HD3	1.80	0.64
1:P:2:ILE:CG2	1:P:3:LYS:H	2.10	0.64
1:B:268:SER:OG	1:B:271:GLU:HG3	1.97	0.63
1:Q:321:ASN:N	1:Q:321:ASN:HD22	1.96	0.63
1:O:66:LYS:CD	1:O:69:PRO:HA	2.29	0.63
1:B:347:ARG:NH2	1:B:358:LEU:HD22	2.11	0.63
1:A:122:HIS:O	1:A:127:ALA:HB3	1.98	0.63
1:O:7:ASN:ND2	1:O:122:HIS:HE1	1.96	0.62
1:O:65:THR:HG22	1:O:66:LYS:N	2.14	0.62
1:P:352:ARG:C	1:P:354:ARG:N	2.57	0.62
1:Q:36:VAL:HG22	3:Q:361:NAD:H2A	1.80	0.62
1:O:98:TRP:CE3	1:O:98:TRP:HA	2.34	0.62
1:O:323:ARG:CG	1:O:323:ARG:NH1	2.60	0.62
1:P:28:ASN:OD1	1:P:28:ASN:N	2.33	0.62
1:P:185:SER:O	1:P:241:LYS:HD2	1.99	0.62
1:Q:320:PRO:O	1:Q:321:ASN:HB2	1.99	0.62
1:O:71:VAL:O	1:O:72:ALA:HB3	2.00	0.61
1:Q:352:ARG:C	1:Q:354:ARG:N	2.57	0.61
1:O:347:ARG:NH2	1:O:358:LEU:CD2	2.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:317:ASN:ND2	1:R:245:MET:HB3	2.15	0.61
1:O:182:PHE:CE1	1:O:267:THR:HG21	2.36	0.61
1:P:46:ALA:O	1:P:50:LYS:HG3	2.00	0.61
1:Q:10:GLY:O	1:Q:12:ILE:N	2.33	0.61
1:R:65:THR:CG2	1:R:66:LYS:H	2.14	0.61
1:R:352:ARG:HG2	1:R:352:ARG:HH11	1.64	0.61
1:A:285:LYS:HG2	1:A:286:ASN:OD1	2.01	0.61
1:O:12:ILE:O	1:O:16:VAL:HG23	2.01	0.61
1:A:352:ARG:C	1:A:354:ARG:N	2.59	0.61
1:P:351:ALA:HB1	1:P:357:LYS:HA	1.83	0.61
1:R:234:VAL:HG12	1:R:235:ILE:HG13	1.83	0.61
1:R:357:LYS:HG2	1:R:358:LEU:N	2.15	0.61
1:B:132:ILE:HD12	1:B:136:ALA:HB2	1.82	0.61
1:O:128:ARG:CG	1:O:128:ARG:NH1	2.49	0.60
1:Q:152:TYR:HD1	1:Q:157:GLN:HG3	1.66	0.60
1:Q:323:ARG:HG3	1:Q:323:ARG:NH1	2.15	0.60
1:A:357:LYS:HG2	1:A:358:LEU:H	1.64	0.60
1:O:312:LYS:O	1:O:316:GLN:HB2	2.02	0.60
1:O:28:ASN:N	1:O:28:ASN:OD1	2.35	0.60
1:O:37:ASP:OD1	3:O:361:NAD:H1B	2.01	0.60
1:P:321:ASN:N	1:P:321:ASN:HD22	1.99	0.60
1:Q:66:LYS:HD3	1:Q:69:PRO:HA	1.83	0.60
1:Q:182:PHE:CD1	1:Q:267:THR:HG21	2.37	0.60
1:O:123:LEU:HA	1:O:127:ALA:O	2.00	0.60
1:R:113:PHE:O	1:R:119:ALA:HB2	2.01	0.60
1:Q:37:ASP:OD1	3:Q:361:NAD:H1B	2.02	0.60
1:R:285:LYS:O	1:R:286:ASN:HB2	2.00	0.60
1:B:352:ARG:C	1:B:354:ARG:H	2.09	0.60
1:P:350:ALA:O	1:P:352:ARG:N	2.34	0.60
1:O:145:MET:HE2	1:O:344:ASP:HB3	1.84	0.59
1:B:37:ASP:OD1	3:B:361:NAD:H1B	2.02	0.59
1:B:71:VAL:O	1:B:72:ALA:HB3	2.02	0.59
1:R:98:TRP:HA	1:R:98:TRP:CE3	2.37	0.59
1:B:292:ASP:O	1:B:312:LYS:NZ	2.35	0.59
1:B:283:TYR:CD1	1:B:284:MET:HG2	2.37	0.59
1:Q:27:GLY:HA3	1:Q:82:HIS:NE2	2.18	0.59
1:A:351:ALA:HB1	1:A:357:LYS:HA	1.86	0.58
1:P:320:PRO:O	1:P:321:ASN:HB2	2.03	0.58
1:A:323:ARG:NH1	1:A:323:ARG:CG	2.60	0.58
1:B:354:ARG:HB2	1:B:354:ARG:HH11	1.67	0.58
1:P:37:ASP:OD1	3:P:361:NAD:H1B	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:2:ILE:HG23	1:R:3:LYS:N	2.18	0.58
1:O:234:VAL:HG12	1:O:235:ILE:HG13	1.86	0.58
1:A:130:VAL:HB	1:A:159:VAL:HG22	1.84	0.58
1:B:123:LEU:HA	1:B:127:ALA:O	2.03	0.58
1:P:65:THR:CG2	1:P:66:LYS:H	2.16	0.58
1:A:2:ILE:HG23	1:A:3:LYS:N	2.13	0.58
1:B:122:HIS:O	1:B:127:ALA:HB3	2.03	0.58
1:Q:71:VAL:O	1:Q:72:ALA:CB	2.51	0.58
1:B:2:ILE:HG23	1:B:3:LYS:N	2.17	0.58
1:O:2:ILE:HG23	1:O:3:LYS:N	2.18	0.58
1:R:312:LYS:O	1:R:316:GLN:HB2	2.04	0.58
1:Q:171:ALA:HB3	1:Q:172:PRO:HD3	1.85	0.58
1:A:156:GLU:OE1	1:A:156:GLU:CA	2.43	0.57
1:B:7:ASN:ND2	1:B:122:HIS:HE1	2.02	0.57
1:B:65:THR:CG2	1:B:66:LYS:N	2.67	0.57
1:Q:65:THR:HG22	1:Q:66:LYS:H	1.67	0.57
1:R:37:ASP:O	1:R:89:ALA:HB2	2.04	0.57
1:R:65:THR:CG2	1:R:66:LYS:N	2.66	0.57
1:A:20:LEU:C	1:A:20:LEU:HD12	2.29	0.57
1:Q:3:LYS:HB3	1:Q:104:GLU:HG2	1.86	0.57
1:Q:78:VAL:HA	1:Q:82:HIS:O	2.04	0.57
1:Q:98:TRP:CE3	1:Q:98:TRP:HA	2.38	0.57
1:Q:71:VAL:O	1:Q:72:ALA:HB3	2.03	0.57
1:B:183:GLY:HA3	1:B:264:THR:HB	1.86	0.57
1:R:37:ASP:OD1	3:R:361:NAD:H1B	2.03	0.57
1:R:351:ALA:HB1	1:R:357:LYS:HA	1.87	0.57
1:P:27:GLY:HA3	1:P:82:HIS:NE2	2.20	0.57
1:O:152:TYR:CD1	1:O:157:GLN:HG3	2.40	0.57
1:Q:352:ARG:HG2	1:Q:352:ARG:HH11	1.68	0.57
1:O:295:LEU:O	1:P:211:ARG:HD3	2.04	0.57
1:A:28:ASN:N	1:A:28:ASN:OD1	2.38	0.56
1:A:65:THR:HG22	1:A:66:LYS:H	1.69	0.56
1:O:182:PHE:CD1	1:O:267:THR:HG21	2.40	0.56
1:R:98:TRP:HA	1:R:98:TRP:HE3	1.69	0.56
1:O:98:TRP:HA	1:O:98:TRP:HE3	1.69	0.56
1:P:225:THR:OG1	2:P:360:SO4:O4	2.20	0.56
1:P:227:ALA:O	1:P:231:VAL:HG23	2.05	0.56
1:P:292:ASP:O	1:P:312:LYS:NZ	2.39	0.56
1:R:2:ILE:O	1:R:31:ASP:N	2.32	0.56
1:O:65:THR:HG22	1:O:66:LYS:H	1.71	0.56
1:Q:63:SER:HB3	1:Q:78:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:175:HIS:O	1:R:179:LYS:HB2	2.06	0.56
1:B:113:PHE:O	1:B:119:ALA:HB2	2.05	0.56
1:O:1:THR:CG2	1:O:30:ILE:HG23	2.35	0.56
1:R:352:ARG:C	1:R:354:ARG:N	2.63	0.56
1:A:350:ALA:O	1:A:352:ARG:N	2.37	0.56
1:Q:235:ILE:HG22	1:Q:238:THR:HG23	1.86	0.56
1:O:277:LYS:O	1:O:280:SER:HB2	2.06	0.56
1:P:98:TRP:HA	1:P:98:TRP:CE3	2.40	0.56
1:R:156:GLU:OE1	1:R:156:GLU:CA	2.46	0.56
1:P:71:VAL:O	1:P:72:ALA:CB	2.53	0.55
1:A:71:VAL:O	1:A:72:ALA:CB	2.54	0.55
1:P:228:ALA:O	1:P:231:VAL:HB	2.05	0.55
1:R:71:VAL:O	1:R:72:ALA:HB3	2.06	0.55
1:A:27:GLY:HA3	1:A:82:HIS:NE2	2.22	0.55
1:R:87:VAL:HG12	1:R:88:LYS:N	2.21	0.55
1:O:71:VAL:O	1:O:72:ALA:CB	2.53	0.55
1:B:28:ASN:OD1	1:B:28:ASN:N	2.39	0.55
1:B:194:SER:HB3	1:B:251:THR:O	2.07	0.55
1:Q:58:PHE:CE2	1:Q:60:HIS:HB2	2.41	0.55
1:Q:1:THR:O	1:Q:2:ILE:HG22	2.07	0.55
1:A:3:LYS:HB3	1:A:104:GLU:HG2	1.89	0.55
1:O:325:PHE:CE1	1:P:325:PHE:HE1	2.23	0.55
1:B:65:THR:CG2	1:B:66:LYS:H	2.20	0.54
1:A:96:LEU:HD12	1:A:98:TRP:CZ2	2.42	0.54
1:A:78:VAL:HA	1:A:82:HIS:O	2.06	0.54
1:B:185:SER:O	1:B:241:LYS:HD2	2.06	0.54
1:Q:38:MET:O	1:Q:39:ASN:HB3	2.08	0.54
1:P:312:LYS:O	1:P:316:GLN:HB2	2.07	0.54
1:A:37:ASP:CG	1:A:38:MET:H	2.15	0.54
1:P:166:THR:HG21	1:P:189:MET:HE1	1.89	0.54
1:P:175:HIS:O	1:P:179:LYS:HB2	2.08	0.54
1:P:302:SER:N	1:P:333:ASP:OD2	2.36	0.54
1:P:352:ARG:HH11	1:P:352:ARG:CG	2.20	0.54
1:A:145:MET:HE2	1:A:344:ASP:HB3	1.90	0.54
1:A:73:LYS:O	1:A:74:ASP:C	2.50	0.54
1:A:348:HIS:CE1	1:A:352:ARG:HH21	2.26	0.54
1:B:37:ASP:O	1:B:89:ALA:HB2	2.08	0.54
1:B:98:TRP:CD1	1:B:127:ALA:HB2	2.42	0.54
1:Q:98:TRP:HA	1:Q:98:TRP:HE3	1.73	0.54
1:Q:113:PHE:O	1:Q:119:ALA:HB2	2.07	0.54
1:B:322:GLU:HG2	1:B:325:PHE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ARG:NH1	1:B:352:ARG:HG2	2.22	0.53
1:P:12:ILE:O	1:P:16:VAL:HG23	2.07	0.53
1:Q:105:TYR:OH	1:Q:350:ALA:HA	2.08	0.53
1:R:22:ASP:C	1:R:24:GLY:H	2.17	0.53
1:A:92:ASN:OD1	1:A:94:ALA:HB3	2.09	0.53
1:Q:96:LEU:HD12	1:Q:98:TRP:CZ2	2.44	0.53
1:Q:172:PRO:HB3	1:Q:284:MET:HE2	1.90	0.53
1:A:65:THR:CG2	1:A:66:LYS:N	2.72	0.53
1:A:185:SER:O	1:A:241:LYS:HD2	2.09	0.53
1:A:357:LYS:HG2	1:A:358:LEU:C	2.34	0.53
1:B:162:ASN:HD22	1:B:342:VAL:HG22	1.74	0.53
1:R:350:ALA:C	1:R:352:ARG:N	2.65	0.53
1:P:37:ASP:C	1:P:89:ALA:HB2	2.33	0.53
1:P:203:ASP:HB2	1:Q:11:ARG:NH1	2.23	0.53
1:Q:141:LYS:HG2	1:Q:143:PHE:CZ	2.44	0.53
1:O:153:ASN:O	1:O:157:GLN:HG2	2.08	0.53
1:P:156:GLU:OE1	1:P:156:GLU:CA	2.53	0.53
1:Q:7:ASN:ND2	1:Q:122:HIS:HE1	2.07	0.53
1:B:37:ASP:CG	1:B:38:MET:H	2.17	0.52
1:B:163:ALA:HB3	1:B:168:ASN:ND2	2.24	0.52
1:O:165:CYS:HB3	3:O:361:NAD:H4N	1.92	0.52
1:R:350:ALA:O	1:R:352:ARG:N	2.42	0.52
1:B:63:SER:HB3	1:B:78:VAL:HB	1.91	0.52
1:B:132:ILE:HD12	1:B:136:ALA:CB	2.39	0.52
1:O:352:ARG:C	1:O:354:ARG:N	2.67	0.52
1:R:153:ASN:CG	1:R:156:GLU:HB2	2.33	0.52
1:A:155:ARG:O	1:A:158:HIS:HE1	1.92	0.52
3:P:361:NAD:O1N	3:P:361:NAD:O2A	2.25	0.52
1:R:28:ASN:N	1:R:28:ASN:OD1	2.42	0.52
1:P:96:LEU:HD12	1:P:98:TRP:CE2	2.44	0.52
1:R:352:ARG:HH11	1:R:352:ARG:CG	2.22	0.52
1:B:10:GLY:O	1:B:12:ILE:N	2.42	0.52
1:B:11:ARG:HG3	3:B:361:NAD:O2A	2.10	0.52
1:Q:347:ARG:NH2	1:Q:358:LEU:CD2	2.73	0.52
1:R:341:ARG:HA	1:R:344:ASP:HB2	1.90	0.52
1:A:66:LYS:HD3	1:A:69:PRO:HA	1.92	0.52
1:A:277:LYS:HA	1:A:290:TYR:CD1	2.45	0.52
1:B:98:TRP:HA	1:B:98:TRP:CE3	2.44	0.52
1:Q:93:PRO:HG3	1:Q:113:PHE:CE1	2.45	0.52
1:B:234:VAL:HG12	1:B:235:ILE:HG13	1.91	0.52
1:A:75:ASP:OD1	1:A:76:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:338:TYR:O	1:O:342:VAL:HG23	2.09	0.52
1:Q:325:PHE:CE2	1:R:188:LEU:HD12	2.45	0.52
1:R:123:LEU:HA	1:R:127:ALA:O	2.10	0.52
1:A:122:HIS:C	1:A:127:ALA:HB3	2.34	0.52
1:B:312:LYS:O	1:B:316:GLN:HB2	2.09	0.52
1:O:27:GLY:HA3	1:O:82:HIS:NE2	2.25	0.52
1:O:301:ILE:O	1:O:302:SER:HB2	2.10	0.52
1:R:71:VAL:O	1:R:72:ALA:CB	2.57	0.52
1:P:50:LYS:HA	1:P:58:PHE:HB2	1.92	0.52
1:A:202:VAL:O	1:A:203:ASP:C	2.52	0.51
1:A:352:ARG:HH11	1:A:352:ARG:CG	2.23	0.51
1:B:71:VAL:O	1:B:72:ALA:CB	2.58	0.51
1:P:235:ILE:HG22	1:P:235:ILE:O	2.10	0.51
1:B:306:SER:OG	1:B:341:ARG:HD2	2.11	0.51
1:A:50:LYS:HG2	1:A:62:VAL:HG21	1.93	0.51
1:A:37:ASP:OD1	3:A:361:NAD:H1B	2.10	0.51
1:O:144:VAL:HG23	1:O:234:VAL:HG21	1.92	0.51
1:B:331:TRP:O	1:B:332:TYR:HB3	2.11	0.51
1:B:163:ALA:HB3	1:B:168:ASN:HD21	1.76	0.51
1:R:89:ALA:HB1	3:R:361:NAD:N1A	2.25	0.51
1:R:347:ARG:HH21	1:R:358:LEU:CD1	2.18	0.51
1:A:110:THR:HG22	3:A:361:NAD:C4A	2.40	0.51
1:Q:152:TYR:CD1	1:Q:157:GLN:HG3	2.45	0.51
1:R:348:HIS:CE1	1:R:352:ARG:HH21	2.29	0.51
1:O:206:SER:HB3	1:O:209:ASP:O	2.11	0.50
1:P:59:LYS:O	1:P:60:HIS:CD2	2.63	0.50
1:O:235:ILE:HG22	1:O:238:THR:HG23	1.93	0.50
1:P:65:THR:CG2	1:P:66:LYS:N	2.70	0.50
1:P:75:ASP:OD1	1:P:76:THR:HG23	2.11	0.50
1:Q:352:ARG:HH11	1:Q:352:ARG:CG	2.23	0.50
1:A:323:ARG:NE	1:R:278:ARG:HH21	2.10	0.50
1:B:50:LYS:HG2	1:B:62:VAL:HG21	1.93	0.50
1:O:1:THR:O	1:O:2:ILE:HG22	2.10	0.50
1:Q:2:ILE:CG2	1:Q:3:LYS:N	2.69	0.50
1:Q:112:LEU:C	1:Q:113:PHE:CD2	2.89	0.50
1:A:1:THR:O	1:A:2:ILE:HG22	2.12	0.50
1:A:153:ASN:O	1:A:157:GLN:HG2	2.11	0.50
1:P:130:VAL:HB	1:P:159:VAL:HG22	1.93	0.50
1:Q:351:ALA:HB1	1:Q:357:LYS:HA	1.93	0.50
1:B:194:SER:OG	1:B:254:VAL:O	2.23	0.50
1:P:172:PRO:HB3	1:P:284:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:232:GLY:O	1:R:236:PRO:HA	2.12	0.50
1:O:325:PHE:CD2	1:P:186:THR:HG23	2.47	0.49
1:O:297:SER:HB3	1:P:220:ILE:HB	1.93	0.49
1:R:350:ALA:O	1:R:351:ALA:C	2.55	0.49
1:A:65:THR:CG2	1:A:66:LYS:H	2.25	0.49
1:B:228:ALA:O	1:B:231:VAL:HB	2.13	0.49
1:O:7:ASN:HD22	1:O:122:HIS:HE1	1.60	0.49
1:O:183:GLY:HA3	1:O:264:THR:HB	1.93	0.49
1:B:73:LYS:O	1:B:74:ASP:C	2.55	0.49
1:B:232:GLY:O	1:B:236:PRO:HA	2.13	0.49
1:Q:28:ASN:OD1	1:Q:28:ASN:N	2.45	0.49
1:A:211:ARG:HG3	1:B:294:GLU:HB3	1.95	0.49
1:P:50:LYS:HG2	1:P:62:VAL:HG21	1.93	0.49
1:Q:294:GLU:HB3	1:R:211:ARG:HG3	1.94	0.49
1:R:87:VAL:CG1	1:R:88:LYS:N	2.75	0.49
1:A:350:ALA:C	1:A:352:ARG:N	2.70	0.49
1:O:110:THR:HG22	3:O:361:NAD:C4A	2.43	0.49
1:R:259:LEU:O	1:R:327:LYS:HA	2.12	0.49
1:A:123:LEU:HA	1:A:127:ALA:O	2.13	0.49
1:Q:183:GLY:HA3	1:Q:264:THR:HB	1.93	0.49
1:Q:222:PRO:HG2	1:R:331:TRP:HZ2	1.77	0.49
1:A:3:LYS:CG	1:A:102:GLY:O	2.60	0.49
1:A:50:LYS:HA	1:A:58:PHE:HB2	1.94	0.49
1:B:225:THR:OG1	2:B:360:SO4:O4	2.17	0.49
1:P:87:VAL:HG12	1:P:88:LYS:N	2.27	0.49
1:P:350:ALA:C	1:P:352:ARG:N	2.71	0.49
1:A:98:TRP:HA	1:A:98:TRP:CE3	2.48	0.48
1:A:134:ALA:HB1	1:A:135:PRO:CD	2.42	0.48
1:B:266:ASP:HB3	1:B:323:ARG:HD2	1.94	0.48
1:Q:37:ASP:CG	3:Q:361:NAD:HO2A	2.19	0.48
1:Q:234:VAL:HG12	1:Q:235:ILE:HG13	1.94	0.48
1:Q:297:SER:HB3	1:R:220:ILE:H	1.78	0.48
1:A:38:MET:O	1:A:39:ASN:CB	2.56	0.48
1:O:164:SER:O	1:O:168:ASN:ND2	2.46	0.48
1:Q:299:ASP:CG	1:R:214:ARG:HH22	2.20	0.48
1:O:75:ASP:OD1	1:O:76:THR:HG23	2.13	0.48
1:O:351:ALA:HB1	1:O:357:LYS:HA	1.93	0.48
1:P:87:VAL:CG1	1:P:88:LYS:N	2.76	0.48
1:A:348:HIS:HE1	1:A:352:ARG:HH21	1.61	0.48
1:B:105:TYR:OH	1:B:350:ALA:HA	2.13	0.48
1:O:66:LYS:HD3	1:O:69:PRO:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:10:GLY:O	1:P:12:ILE:N	2.47	0.48
1:P:98:TRP:HA	1:P:98:TRP:HE3	1.77	0.48
1:P:187:GLY:HA3	1:P:242:LEU:HD23	1.96	0.48
1:R:225:THR:HG22	1:R:245:MET:HA	1.96	0.48
1:A:10:GLY:HA2	1:A:14:ARG:HG3	1.96	0.48
1:A:350:ALA:O	1:A:351:ALA:C	2.56	0.48
1:O:96:LEU:HD12	1:O:98:TRP:CZ2	2.48	0.48
1:R:301:ILE:O	1:R:302:SER:HB2	2.13	0.48
1:O:238:THR:HA	1:O:241:LYS:HE2	1.96	0.48
1:O:284:MET:HB3	1:O:284:MET:HE3	1.55	0.48
1:O:325:PHE:HE1	1:P:325:PHE:CE1	2.26	0.48
1:Q:1:THR:HA	1:Q:350:ALA:HB1	1.95	0.48
1:A:1:THR:HG21	1:A:30:ILE:HD13	1.95	0.48
1:B:58:PHE:CE2	1:B:60:HIS:HB2	2.49	0.48
1:B:78:VAL:HA	1:B:82:HIS:O	2.14	0.48
1:O:297:SER:OG	1:P:219:ASN:HA	2.14	0.48
1:R:171:ALA:HB3	1:R:172:PRO:HD3	1.95	0.48
1:B:255:SER:HB2	1:B:332:TYR:CZ	2.49	0.48
1:O:2:ILE:CG2	1:O:3:LYS:H	2.24	0.48
1:Q:65:THR:CG2	1:Q:66:LYS:N	2.76	0.48
1:R:348:HIS:HE1	1:R:352:ARG:HH21	1.60	0.48
1:R:207:VAL:O	1:R:207:VAL:HG22	2.13	0.48
1:O:153:ASN:H	1:O:157:GLN:HE21	1.61	0.47
1:O:348:HIS:CE1	1:O:352:ARG:HH21	2.32	0.47
1:B:98:TRP:HA	1:B:98:TRP:HE3	1.77	0.47
1:B:120:GLU:HG3	1:B:159:VAL:HG21	1.95	0.47
1:B:350:ALA:O	1:B:355:ALA:HB3	2.14	0.47
1:P:145:MET:HE2	1:P:344:ASP:HB3	1.96	0.47
1:Q:20:LEU:C	1:Q:20:LEU:HD12	2.39	0.47
1:R:78:VAL:HA	1:R:82:HIS:O	2.14	0.47
1:R:348:HIS:CE1	1:R:352:ARG:NH2	2.82	0.47
1:B:253:ASP:C	1:B:254:VAL:HG23	2.38	0.47
1:A:348:HIS:CE1	1:A:352:ARG:NH2	2.83	0.47
1:Q:182:PHE:HD1	1:Q:267:THR:HG21	1.80	0.47
1:B:352:ARG:C	1:B:354:ARG:N	2.69	0.47
1:O:17:PHE:O	1:O:20:LEU:HG	2.14	0.47
1:Q:348:HIS:CE1	1:Q:352:ARG:HH21	2.32	0.47
1:A:2:ILE:CG2	1:A:3:LYS:H	2.18	0.47
1:A:282:THR:HB	1:A:283:TYR:H	1.56	0.47
1:B:120:GLU:HG2	1:B:123:LEU:HD12	1.97	0.47
1:B:268:SER:HG	1:B:271:GLU:HG3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ARG:HG2	1:B:352:ARG:HH11	1.79	0.47
1:O:173:LEU:HD21	1:O:330:SER:HB2	1.96	0.47
1:Q:141:LYS:HG2	1:Q:143:PHE:CE2	2.49	0.47
1:Q:357:LYS:HE3	1:Q:358:LEU:C	2.39	0.47
1:B:348:HIS:CE1	1:B:352:ARG:HH21	2.33	0.47
1:O:348:HIS:CE1	1:O:352:ARG:NH2	2.83	0.47
1:O:352:ARG:HH11	1:O:352:ARG:CG	2.22	0.47
1:Q:297:SER:HB3	1:R:220:ILE:HB	1.97	0.47
1:B:351:ALA:HB1	1:B:357:LYS:HA	1.97	0.47
1:P:350:ALA:C	1:P:352:ARG:H	2.22	0.47
1:B:182:PHE:CE1	1:B:267:THR:HG21	2.50	0.46
1:P:59:LYS:HA	1:P:59:LYS:HD3	1.72	0.46
1:A:3:LYS:HG2	1:A:102:GLY:O	2.15	0.46
1:P:202:VAL:O	1:P:203:ASP:C	2.58	0.46
1:Q:255:SER:HB2	1:Q:332:TYR:CZ	2.51	0.46
1:R:350:ALA:C	1:R:352:ARG:H	2.24	0.46
1:A:350:ALA:C	1:A:352:ARG:H	2.24	0.46
1:O:44:TYR:O	1:O:48:GLN:HG3	2.15	0.46
1:A:189:MET:O	1:A:189:MET:HG3	2.16	0.46
1:A:259:LEU:O	1:A:327:LYS:HA	2.15	0.46
1:P:73:LYS:O	1:P:74:ASP:C	2.58	0.46
1:R:153:ASN:OD1	1:R:155:ARG:HB3	2.16	0.46
1:O:66:LYS:HD2	1:O:69:PRO:HA	1.96	0.46
1:P:38:MET:HB3	1:P:38:MET:HE3	1.60	0.46
1:A:45:PHE:HB3	1:A:77:LEU:HD21	1.97	0.46
1:B:122:HIS:C	1:B:127:ALA:HB3	2.39	0.46
1:O:73:LYS:O	1:O:74:ASP:C	2.58	0.46
1:O:78:VAL:HA	1:O:82:HIS:O	2.16	0.46
1:R:228:ALA:O	1:R:229:LYS:C	2.58	0.46
1:B:352:ARG:HH11	1:B:352:ARG:CG	2.29	0.46
1:B:354:ARG:HH11	1:B:354:ARG:N	2.14	0.46
1:R:225:THR:OG1	2:R:360:SO4:O1	2.30	0.46
1:A:153:ASN:H	1:A:157:GLN:CG	2.29	0.46
1:A:290:TYR:C	1:A:290:TYR:CD2	2.94	0.46
1:A:217:ALA:HA	1:A:250:PRO:HB3	1.98	0.46
1:O:268:SER:OG	1:O:271:GLU:HG3	2.15	0.46
1:Q:1:THR:HA	1:Q:350:ALA:CB	2.46	0.46
1:Q:348:HIS:HE1	1:Q:352:ARG:HH21	1.62	0.46
1:R:283:TYR:CE1	1:R:284:MET:HG2	2.51	0.46
1:B:347:ARG:NH2	1:B:358:LEU:CD2	2.79	0.46
1:O:313:ALA:O	1:O:317:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:THR:HG23	1:A:136:ALA:HA	1.99	0.45
1:O:323:ARG:O	1:O:324:ARG:HD3	2.16	0.45
1:P:92:ASN:HA	1:P:93:PRO:HD3	1.76	0.45
1:P:113:PHE:O	1:P:119:ALA:HB2	2.16	0.45
1:R:73:LYS:O	1:R:74:ASP:C	2.59	0.45
1:R:238:THR:HA	1:R:241:LYS:HE2	1.98	0.45
1:P:177:LEU:HD23	1:P:177:LEU:HA	1.83	0.45
1:P:351:ALA:CB	1:P:357:LYS:HA	2.46	0.45
1:Q:3:LYS:HA	1:Q:3:LYS:HD3	1.74	0.45
1:Q:41:ASP:O	1:Q:45:PHE:HD1	2.00	0.45
1:O:65:THR:CG2	1:O:66:LYS:N	2.80	0.45
1:O:113:PHE:O	1:O:119:ALA:HB2	2.17	0.45
1:O:282:THR:O	1:O:285:LYS:HB2	2.16	0.45
1:B:153:ASN:OD1	1:B:153:ASN:C	2.60	0.45
1:P:4:VAL:HG12	1:P:5:GLY:N	2.31	0.45
1:A:34:ALA:HB1	1:A:85:LEU:O	2.17	0.45
1:B:11:ARG:O	1:B:15:MET:CG	2.58	0.45
1:B:173:LEU:HD12	1:B:173:LEU:HA	1.54	0.45
1:B:284:MET:HE3	1:B:284:MET:HB3	1.77	0.45
1:R:327:LYS:O	1:R:327:LYS:HG3	2.10	0.45
1:B:44:TYR:O	1:B:48:GLN:HG3	2.16	0.45
1:P:110:THR:HG22	3:P:361:NAD:C4A	2.47	0.45
1:A:153:ASN:H	1:A:157:GLN:HG3	1.81	0.45
1:B:228:ALA:O	1:B:229:LYS:C	2.60	0.45
1:O:67:SER:OG	1:O:68:LYS:N	2.46	0.45
1:O:210:TRP:HB3	1:R:47:TYR:CE2	2.52	0.45
1:Q:37:ASP:O	1:Q:89:ALA:HB2	2.16	0.45
1:Q:129:LYS:HE3	1:Q:152:TYR:OH	2.16	0.45
1:A:59:LYS:HA	1:A:59:LYS:HD3	1.72	0.45
1:O:92:ASN:HA	1:O:93:PRO:HD3	1.83	0.45
1:P:182:PHE:CE1	1:P:267:THR:HG21	2.51	0.45
1:Q:182:PHE:CE1	1:Q:267:THR:HG21	2.52	0.45
1:R:38:MET:HE3	1:R:38:MET:HB3	1.66	0.45
1:A:277:LYS:HG2	1:A:290:TYR:CZ	2.52	0.45
1:B:179:LYS:C	1:B:181:GLY:N	2.73	0.45
1:O:340:HIS:O	1:O:341:ARG:C	2.59	0.45
1:Q:357:LYS:HE3	1:Q:358:LEU:OXT	2.17	0.45
1:B:269:ILE:HG23	1:B:315:LEU:HD23	1.98	0.44
1:R:153:ASN:HB3	1:R:156:GLU:HB2	1.98	0.44
1:R:211:ARG:O	1:R:221:ILE:HG21	2.17	0.44
1:A:92:ASN:HA	1:A:93:PRO:HD3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:211:ARG:HD3	1:P:295:LEU:O	2.17	0.44
1:Q:92:ASN:HA	1:Q:93:PRO:HD3	1.77	0.44
1:A:135:PRO:HG3	1:A:164:SER:HB3	1.98	0.44
1:A:357:LYS:CG	1:A:358:LEU:N	2.62	0.44
1:B:270:LYS:HB3	1:B:270:LYS:HE3	1.55	0.44
1:O:37:ASP:CG	1:O:38:MET:H	2.26	0.44
1:O:290:TYR:C	1:O:290:TYR:CD2	2.95	0.44
1:R:230:ALA:O	1:R:233:MET:HB2	2.17	0.44
1:O:87:VAL:HG12	1:O:88:LYS:N	2.32	0.44
1:O:354:ARG:HE	1:O:354:ARG:HB2	1.59	0.44
1:O:348:HIS:HE1	1:O:352:ARG:HH21	1.65	0.44
1:Q:122:HIS:HB2	1:Q:130:VAL:HG21	2.00	0.44
1:B:12:ILE:HD13	1:B:12:ILE:HA	1.87	0.44
1:P:268:SER:OG	1:P:271:GLU:HG3	2.17	0.44
1:Q:3:LYS:CB	1:Q:104:GLU:HG2	2.47	0.44
1:Q:66:LYS:CD	1:Q:69:PRO:HA	2.48	0.44
1:R:314:THR:O	1:R:318:ASN:ND2	2.49	0.44
1:A:120:GLU:HG2	1:A:123:LEU:HD12	1.99	0.44
1:A:351:ALA:CB	1:A:357:LYS:HA	2.46	0.44
1:R:37:ASP:C	1:R:89:ALA:HB2	2.43	0.44
1:R:145:MET:HE2	1:R:344:ASP:HB3	1.99	0.44
1:R:333:ASP:OD1	1:R:333:ASP:C	2.60	0.44
1:R:2:ILE:CG2	1:R:3:LYS:H	2.28	0.44
1:B:230:ALA:O	1:B:233:MET:HB2	2.18	0.44
1:B:238:THR:HA	1:B:241:LYS:HE2	1.99	0.44
1:O:128:ARG:HG2	1:O:128:ARG:O	2.18	0.44
1:P:187:GLY:C	1:P:242:LEU:HD23	2.42	0.44
1:Q:98:TRP:CD1	1:Q:127:ALA:HB2	2.52	0.44
1:Q:110:THR:HG22	3:Q:361:NAD:C4A	2.48	0.44
1:R:110:THR:HG22	3:R:361:NAD:C4A	2.47	0.44
1:R:153:ASN:H	1:R:157:GLN:HE21	1.63	0.44
1:A:228:ALA:O	1:A:231:VAL:HB	2.18	0.43
1:A:350:ALA:C	1:A:355:ALA:HB3	2.43	0.43
1:O:320:PRO:O	1:O:321:ASN:HB2	2.17	0.43
1:P:232:GLY:O	1:P:236:PRO:HA	2.18	0.43
1:O:269:ILE:HD12	1:O:269:ILE:HA	1.90	0.43
1:P:1:THR:HG22	1:P:30:ILE:HG12	2.00	0.43
1:P:4:VAL:CG1	1:P:5:GLY:N	2.81	0.43
1:A:270:LYS:HB3	1:A:270:LYS:HE3	1.70	0.43
1:B:141:LYS:HG2	1:B:143:PHE:CZ	2.53	0.43
1:Q:97:PRO:HG2	1:Q:101:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:88:LYS:HA	1:R:88:LYS:HD2	1.89	0.43
1:A:191:THR:O	1:A:191:THR:HG23	2.18	0.43
1:A:207:VAL:O	1:A:207:VAL:HG22	2.17	0.43
1:Q:345:LEU:O	1:Q:349:MET:HG3	2.19	0.43
1:R:38:MET:O	1:R:39:ASN:CB	2.60	0.43
1:R:153:ASN:C	1:R:155:ARG:N	2.76	0.43
1:Q:93:PRO:CG	1:Q:113:PHE:CE1	3.01	0.43
1:Q:350:ALA:C	1:Q:355:ALA:HB3	2.43	0.43
1:A:153:ASN:ND2	1:A:156:GLU:HB2	2.33	0.43
1:O:93:PRO:HG3	1:O:113:PHE:CD1	2.53	0.43
1:O:152:TYR:HD1	1:O:157:GLN:HG3	1.80	0.43
1:R:350:ALA:C	1:R:355:ALA:HB3	2.43	0.43
1:A:152:TYR:CD1	1:A:157:GLN:HG3	2.54	0.43
1:B:132:ILE:HG13	1:B:160:VAL:O	2.18	0.43
1:O:37:ASP:C	1:O:39:ASN:H	2.27	0.43
1:P:11:ARG:HH12	1:Q:203:ASP:HB2	1.83	0.43
1:Q:93:PRO:HD3	1:Q:113:PHE:CE1	2.54	0.43
1:R:236:PRO:C	1:R:238:THR:N	2.77	0.43
1:A:152:TYR:HD1	1:A:157:GLN:HG3	1.83	0.43
1:B:179:LYS:C	1:B:181:GLY:H	2.26	0.43
1:O:65:THR:CG2	1:O:66:LYS:H	2.32	0.43
1:R:162:ASN:O	1:R:163:ALA:HB3	2.18	0.43
1:B:63:SER:O	1:B:78:VAL:N	2.45	0.43
1:Q:22:ASP:C	1:Q:24:GLY:H	2.26	0.43
1:Q:157:GLN:H	1:Q:157:GLN:HG2	1.66	0.43
1:A:232:GLY:O	1:A:236:PRO:HA	2.19	0.42
1:P:283:TYR:H	1:P:283:TYR:HD2	1.64	0.42
1:Q:45:PHE:HB3	1:Q:77:LEU:HD21	2.00	0.42
1:P:206:SER:HB3	1:P:209:ASP:O	2.18	0.42
1:R:152:TYR:CD1	1:R:157:GLN:HG3	2.54	0.42
1:B:122:HIS:HB2	1:B:130:VAL:HG21	2.01	0.42
1:O:347:ARG:HH22	1:O:358:LEU:CD2	2.30	0.42
1:R:1:THR:O	1:R:2:ILE:HG22	2.19	0.42
1:R:11:ARG:O	1:R:15:MET:CG	2.60	0.42
1:O:235:ILE:HG22	1:O:235:ILE:O	2.19	0.42
1:P:73:LYS:HB3	1:P:73:LYS:HE2	1.71	0.42
1:P:189:MET:O	1:P:244:GLY:HA3	2.19	0.42
1:P:205:VAL:HG22	1:Q:48:GLN:HE22	1.84	0.42
1:P:285:LYS:HG2	1:P:286:ASN:OD1	2.20	0.42
1:Q:156:GLU:OE1	1:Q:156:GLU:CA	2.53	0.42
1:Q:268:SER:OG	1:Q:271:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:MET:HE1	1:A:227:ALA:HB3	2.01	0.42
1:B:1:THR:CG2	1:B:30:ILE:HG23	2.50	0.42
1:B:267:THR:HB	1:B:268:SER:H	1.63	0.42
1:B:267:THR:HG22	1:B:271:GLU:OE1	2.20	0.42
1:P:88:LYS:HD2	1:P:88:LYS:HA	1.83	0.42
1:P:106:VAL:HG12	1:P:127:ALA:HB1	2.01	0.42
1:Q:285:LYS:HG2	1:Q:286:ASN:OD1	2.20	0.42
1:Q:358:LEU:HD12	1:Q:358:LEU:HA	1.91	0.42
1:A:122:HIS:HB2	1:A:130:VAL:HG21	2.02	0.42
1:B:143:PHE:CZ	1:B:152:TYR:HA	2.55	0.42
1:B:350:ALA:C	1:B:355:ALA:HB3	2.45	0.42
1:P:11:ARG:O	1:P:15:MET:N	2.51	0.42
1:A:173:LEU:HD12	1:A:173:LEU:HA	1.88	0.42
1:A:239:GLN:HE21	1:A:239:GLN:HB2	1.62	0.42
1:B:10:GLY:HA2	1:B:14:ARG:HG3	2.00	0.42
1:P:172:PRO:HB3	1:P:284:MET:CE	2.50	0.42
1:R:92:ASN:OD1	1:R:94:ALA:HB3	2.19	0.42
1:R:188:LEU:O	1:R:259:LEU:HD12	2.20	0.42
1:A:98:TRP:HA	1:A:98:TRP:HE3	1.84	0.42
1:O:46:ALA:O	1:O:50:LYS:HG3	2.20	0.42
1:Q:333:ASP:OD1	1:Q:333:ASP:C	2.63	0.42
1:R:348:HIS:O	1:R:352:ARG:HB2	2.20	0.42
1:B:333:ASP:OD1	1:B:333:ASP:C	2.63	0.42
1:P:78:VAL:HA	1:P:82:HIS:O	2.20	0.42
1:O:173:LEU:HD12	1:O:173:LEU:HA	1.63	0.42
1:P:262:ILE:HA	1:P:324:ARG:O	2.20	0.42
1:P:303:ASP:OD1	1:P:303:ASP:C	2.63	0.42
1:Q:173:LEU:HD21	1:Q:330:SER:HB2	2.02	0.42
1:A:277:LYS:HG2	1:A:290:TYR:CE1	2.55	0.41
1:P:111:GLY:C	1:P:112:LEU:HD12	2.45	0.41
1:R:96:LEU:HD12	1:R:98:TRP:CZ2	2.55	0.41
1:A:183:GLY:C	1:A:184:ILE:HG12	2.45	0.41
1:B:93:PRO:HD3	1:B:113:PHE:CE1	2.56	0.41
1:O:104:GLU:HG3	1:O:105:TYR:CD2	2.55	0.41
1:O:205:VAL:HG22	1:R:48:GLN:HE22	1.85	0.41
1:O:292:ASP:O	1:O:312:LYS:NZ	2.50	0.41
1:Q:92:ASN:OD1	1:Q:94:ALA:HB3	2.20	0.41
1:R:191:THR:O	1:R:191:THR:HG23	2.19	0.41
1:R:351:ALA:CB	1:R:357:LYS:HA	2.48	0.41
1:A:174:VAL:HG13	1:A:184:ILE:CD1	2.50	0.41
1:R:261:PHE:CE1	1:R:326:PHE:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:THR:HG22	1:A:30:ILE:HG12	2.02	0.41
1:A:1:THR:CG2	1:A:30:ILE:HD13	2.50	0.41
1:O:185:SER:O	1:O:241:LYS:HD2	2.21	0.41
1:O:207:VAL:O	1:O:207:VAL:HG22	2.20	0.41
1:P:1:THR:CG2	1:P:30:ILE:HG23	2.50	0.41
1:P:287:ILE:HD13	1:P:287:ILE:HA	1.78	0.41
1:A:23:ASP:HB2	1:A:25:LEU:CD1	2.50	0.41
1:B:2:ILE:O	1:B:31:ASP:N	2.53	0.41
1:B:157:GLN:H	1:B:157:GLN:HG2	1.68	0.41
1:B:353:ASP:C	1:B:355:ALA:N	2.77	0.41
1:O:3:LYS:HA	1:O:3:LYS:HD2	1.76	0.41
1:O:351:ALA:CB	1:O:357:LYS:HA	2.50	0.41
1:P:320:PRO:O	1:P:321:ASN:CB	2.68	0.41
1:Q:193:HIS:ND1	1:Q:194:SER:O	2.52	0.41
1:Q:321:ASN:N	1:Q:321:ASN:ND2	2.67	0.41
1:B:321:ASN:N	1:B:321:ASN:ND2	2.62	0.41
1:O:121:GLY:O	1:O:124:ARG:N	2.54	0.41
1:P:153:ASN:HD22	1:P:156:GLU:HG2	1.82	0.41
1:A:357:LYS:HB3	1:A:357:LYS:HE2	1.58	0.41
1:B:170:LEU:O	1:B:173:LEU:HB2	2.20	0.41
1:O:147:VAL:HG11	1:O:234:VAL:CG1	2.50	0.41
1:P:153:ASN:O	1:P:157:GLN:HG2	2.21	0.41
1:P:179:LYS:HE2	1:P:179:LYS:HB3	1.96	0.41
1:Q:59:LYS:HA	1:Q:59:LYS:HD3	1.85	0.41
1:Q:172:PRO:HB3	1:Q:284:MET:CE	2.51	0.41
1:Q:348:HIS:CE1	1:Q:352:ARG:NH2	2.88	0.41
1:R:12:ILE:O	1:R:16:VAL:HG23	2.21	0.41
1:A:93:PRO:HG3	1:A:113:PHE:CE1	2.56	0.41
3:B:361:NAD:O2A	3:B:361:NAD:O1N	2.38	0.41
1:O:180:GLU:OE1	1:O:278:ARG:NH2	2.41	0.41
1:O:350:ALA:O	1:O:355:ALA:HB3	2.20	0.41
1:P:270:LYS:HD2	1:P:270:LYS:HA	1.90	0.41
1:R:306:SER:OG	1:R:341:ARG:HD2	2.20	0.41
1:B:59:LYS:HD3	1:B:59:LYS:HA	1.81	0.41
1:B:66:LYS:HB3	1:B:66:LYS:HE3	1.69	0.41
1:B:173:LEU:HD21	1:B:330:SER:HB2	2.03	0.41
1:O:117:SER:O	1:O:118:ALA:C	2.64	0.41
1:P:101:LEU:HD12	1:P:101:LEU:HA	1.97	0.41
1:R:120:GLU:HG2	1:R:123:LEU:HD12	2.03	0.41
1:P:296:VAL:O	1:P:297:SER:C	2.63	0.41
1:R:63:SER:HB3	1:R:78:VAL:HB	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:177:LEU:HD23	1:R:177:LEU:HA	1.88	0.41
1:A:269:ILE:HD12	1:A:269:ILE:HA	1.87	0.40
1:O:203:ASP:HB2	1:R:11:ARG:NH1	2.36	0.40
1:O:325:PHE:CD2	1:P:186:THR:CG2	3.04	0.40
1:R:93:PRO:HG3	1:R:113:PHE:CD1	2.56	0.40
1:P:350:ALA:O	1:P:351:ALA:C	2.64	0.40
1:Q:325:PHE:HE1	1:R:325:PHE:HE1	1.69	0.40
1:R:97:PRO:HG2	1:R:101:LEU:HD22	2.03	0.40
1:B:105:TYR:CD1	1:B:129:LYS:HB2	2.57	0.40
1:P:267:THR:HB	1:P:268:SER:H	1.37	0.40
1:Q:270:LYS:HB3	1:Q:270:LYS:HE3	1.56	0.40
1:R:23:ASP:C	1:R:25:LEU:HD12	2.47	0.40
1:R:314:THR:HG23	1:R:327:LYS:O	2.22	0.40
1:B:50:LYS:HB3	1:B:50:LYS:HE3	1.85	0.40
1:P:148:ASN:C	1:P:150:ASN:H	2.30	0.40
1:P:343:VAL:O	1:P:347:ARG:HG3	2.21	0.40
1:A:37:ASP:C	1:A:39:ASN:H	2.29	0.40
1:P:2:ILE:O	1:P:31:ASP:N	2.44	0.40
1:P:269:ILE:HD12	1:P:269:ILE:HA	1.91	0.40
1:P:294:GLU:OE2	1:P:312:LYS:HD2	2.22	0.40
1:R:37:ASP:CG	1:R:38:MET:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/359 (99%)	309 (87%)	35 (10%)	12 (3%)	3	20
1	B	356/359 (99%)	308 (86%)	38 (11%)	10 (3%)	4	25
1	O	356/359 (99%)	305 (86%)	39 (11%)	12 (3%)	3	20
1	P	356/359 (99%)	306 (86%)	39 (11%)	11 (3%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	356/359 (99%)	308 (86%)	36 (10%)	12 (3%)	3	20
1	R	356/359 (99%)	303 (85%)	45 (13%)	8 (2%)	5	29
All	All	2136/2154 (99%)	1839 (86%)	232 (11%)	65 (3%)	3	23

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	72	ALA
1	A	351	ALA
1	A	356	ALA
1	B	11	ARG
1	B	39	ASN
1	B	72	ALA
1	O	11	ARG
1	O	72	ALA
1	O	356	ALA
1	P	72	ALA
1	P	351	ALA
1	P	354	ARG
1	Q	11	ARG
1	Q	72	ALA
1	R	72	ALA
1	A	2	ILE
1	A	254	VAL
1	B	2	ILE
1	B	254	VAL
1	B	354	ARG
1	B	356	ALA
1	O	2	ILE
1	O	74	ASP
1	O	230	ALA
1	O	254	VAL
1	O	351	ALA
1	P	2	ILE
1	P	11	ARG
1	P	254	VAL
1	P	356	ALA
1	Q	2	ILE
1	Q	24	GLY
1	Q	254	VAL

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Mol	Chain	Res	Type
1	Q	356	ALA
1	R	2	ILE
1	R	24	GLY
1	R	39	ASN
1	R	254	VAL
1	R	351	ALA
1	R	356	ALA
1	A	354	ARG
1	B	74	ASP
1	O	39	ASN
1	O	354	ARG
1	P	39	ASN
1	P	67	SER
1	Q	19	ALA
1	Q	39	ASN
1	A	24	GLY
1	A	229	LYS
1	A	357	LYS
1	O	67	SER
1	P	353	ASP
1	Q	89	ALA
1	Q	314	THR
1	Q	353	ASP
1	R	74	ASP
1	A	74	ASP
1	A	350	ALA
1	B	24	GLY
1	B	351	ALA
1	P	350	ALA
1	Q	148	ASN
1	O	237	SER

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/296 (100%)	249 (84%)	46 (16%)	2	13
1	B	295/296 (100%)	250 (85%)	45 (15%)	3	14
1	O	295/296 (100%)	253 (86%)	42 (14%)	3	17
1	P	295/296 (100%)	254 (86%)	41 (14%)	3	17
1	Q	295/296 (100%)	255 (86%)	40 (14%)	3	18
1	R	295/296 (100%)	253 (86%)	42 (14%)	3	17
All	All	1770/1776 (100%)	1514 (86%)	256 (14%)	3	16

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	LYS
1	A	28	ASN
1	A	30	ILE
1	A	36	VAL
1	A	40	THR
1	A	43	ARG
1	A	57	LYS
1	A	62	VAL
1	A	63	SER
1	A	71	VAL
1	A	77	LEU
1	A	96	LEU
1	A	101	LEU
1	A	106	VAL
1	A	114	THR
1	A	115	VAL
1	A	155	ARG
1	A	156	GLU
1	A	157	GLN
1	A	173	LEU
1	A	176	VAL
1	A	184	ILE
1	A	186	THR
1	A	189	MET
1	A	190	THR
1	A	199	GLN

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Mol	Chain	Res	Type
1	A	211	ARG
1	A	225	THR
1	A	229	LYS
1	A	234	VAL
1	A	239	GLN
1	A	256	VAL
1	A	264	THR
1	A	267	THR
1	A	278	ARG
1	A	282	THR
1	A	290	TYR
1	A	316	GLN
1	A	321	ASN
1	A	323	ARG
1	A	334	ASN
1	A	346	VAL
1	A	352	ARG
1	A	357	LYS
1	A	358	LEU
1	B	28	ASN
1	B	30	ILE
1	B	36	VAL
1	B	40	THR
1	B	50	LYS
1	B	62	VAL
1	B	66	LYS
1	B	71	VAL
1	B	73	LYS
1	B	77	LEU
1	B	96	LEU
1	B	101	LEU
1	B	103	VAL
1	B	106	VAL
1	B	114	THR
1	B	115	VAL
1	B	120	GLU
1	B	130	VAL
1	B	149	HIS
1	B	155	ARG
1	B	156	GLU
1	B	157	GLN
1	B	173	LEU

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Mol	Chain	Res	Type
1	B	176	VAL
1	B	179	LYS
1	B	184	ILE
1	B	186	THR
1	B	189	MET
1	B	190	THR
1	B	191	THR
1	B	199	GLN
1	B	211	ARG
1	B	225	THR
1	B	229	LYS
1	B	234	VAL
1	B	264	THR
1	B	267	THR
1	B	281	LYS
1	B	282	THR
1	B	316	GLN
1	B	321	ASN
1	B	327	LYS
1	B	343	VAL
1	B	352	ARG
1	B	354	ARG
1	O	2	ILE
1	O	3	LYS
1	O	28	ASN
1	O	36	VAL
1	O	38	MET
1	O	40	THR
1	O	43	ARG
1	O	62	VAL
1	O	66	LYS
1	O	71	VAL
1	O	73	LYS
1	O	77	LEU
1	O	96	LEU
1	O	101	LEU
1	O	106	VAL
1	O	114	THR
1	O	115	VAL
1	O	117	SER
1	O	128	ARG
1	O	149	HIS

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Mol	Chain	Res	Type
1	O	155	ARG
1	O	156	GLU
1	O	157	GLN
1	O	161	SER
1	O	173	LEU
1	O	179	LYS
1	O	184	ILE
1	O	189	MET
1	O	199	GLN
1	O	218	LEU
1	O	234	VAL
1	O	239	GLN
1	O	256	VAL
1	O	264	THR
1	O	267	THR
1	O	268	SER
1	O	316	GLN
1	O	321	ASN
1	O	323	ARG
1	O	327	LYS
1	O	346	VAL
1	O	352	ARG
1	P	3	LYS
1	P	28	ASN
1	P	36	VAL
1	P	38	MET
1	P	40	THR
1	P	43	ARG
1	P	62	VAL
1	P	66	LYS
1	P	71	VAL
1	P	73	LYS
1	P	76	THR
1	P	77	LEU
1	P	96	LEU
1	P	101	LEU
1	P	106	VAL
1	P	114	THR
1	P	115	VAL
1	P	155	ARG
1	P	156	GLU
1	P	157	GLN

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Mol	Chain	Res	Type
1	P	173	LEU
1	P	176	VAL
1	P	179	LYS
1	P	184	ILE
1	P	186	THR
1	P	189	MET
1	P	199	GLN
1	P	229	LYS
1	P	234	VAL
1	P	239	GLN
1	P	264	THR
1	P	267	THR
1	P	278	ARG
1	P	281	LYS
1	P	282	THR
1	P	316	GLN
1	P	321	ASN
1	P	323	ARG
1	P	327	LYS
1	P	352	ARG
1	P	358	LEU
1	Q	3	LYS
1	Q	28	ASN
1	Q	29	GLU
1	Q	30	ILE
1	Q	36	VAL
1	Q	40	THR
1	Q	50	LYS
1	Q	62	VAL
1	Q	71	VAL
1	Q	73	LYS
1	Q	77	LEU
1	Q	96	LEU
1	Q	101	LEU
1	Q	106	VAL
1	Q	109	SER
1	Q	114	THR
1	Q	115	VAL
1	Q	155	ARG
1	Q	156	GLU
1	Q	157	GLN
1	Q	173	LEU

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Mol	Chain	Res	Type
1	Q	176	VAL
1	Q	184	ILE
1	Q	186	THR
1	Q	199	GLN
1	Q	202	VAL
1	Q	211	ARG
1	Q	229	LYS
1	Q	243	THR
1	Q	264	THR
1	Q	267	THR
1	Q	270	LYS
1	Q	282	THR
1	Q	316	GLN
1	Q	321	ASN
1	Q	323	ARG
1	Q	327	LYS
1	Q	352	ARG
1	Q	354	ARG
1	Q	357	LYS
1	R	3	LYS
1	R	28	ASN
1	R	36	VAL
1	R	38	MET
1	R	40	THR
1	R	62	VAL
1	R	66	LYS
1	R	71	VAL
1	R	73	LYS
1	R	76	THR
1	R	77	LEU
1	R	96	LEU
1	R	101	LEU
1	R	106	VAL
1	R	114	THR
1	R	115	VAL
1	R	120	GLU
1	R	156	GLU
1	R	157	GLN
1	R	173	LEU
1	R	176	VAL
1	R	179	LYS
1	R	184	ILE

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Mol	Chain	Res	Type
1	R	186	THR
1	R	189	MET
1	R	191	THR
1	R	199	GLN
1	R	229	LYS
1	R	234	VAL
1	R	242	LEU
1	R	264	THR
1	R	265	ARG
1	R	267	THR
1	R	282	THR
1	R	287	ILE
1	R	316	GLN
1	R	321	ASN
1	R	323	ARG
1	R	327	LYS
1	R	352	ARG
1	R	354	ARG
1	R	357	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	158	HIS
1	A	175	HIS
1	A	239	GLN
1	A	321	ASN
1	B	7	ASN
1	B	157	GLN
1	B	162	ASN
1	B	321	ASN
1	B	348	HIS
1	O	48	GLN
1	O	157	GLN
1	O	158	HIS
1	O	168	ASN
1	O	286	ASN
1	O	321	ASN
1	O	348	HIS
1	P	317	ASN
1	P	321	ASN

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Mol	Chain	Res	Type
1	Q	48	GLN
1	Q	148	ASN
1	Q	158	HIS
1	Q	321	ASN
1	R	48	GLN
1	R	60	HIS
1	R	157	GLN
1	R	321	ASN
1	R	340	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](#)

18 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	NAD	A	361	-	46,48,48	1.84	7 (15%)	64,73,73	2.15	15 (23%)
3	NAD	P	361	-	46,48,48	1.87	8 (17%)	64,73,73	2.27	19 (29%)
3	NAD	Q	361	-	46,48,48	1.88	7 (15%)	64,73,73	2.14	12 (18%)
2	SO4	R	359	-	4,4,4	0.24	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	R	361	-	46,48,48	1.93	9 (19%)	64,73,73	2.35	16 (25%)
2	SO4	B	359	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	A	359	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	A	360	-	4,4,4	0.27	0	6,6,6	0.29	0
3	NAD	O	361	-	46,48,48	1.94	10 (21%)	64,73,73	2.33	17 (26%)
2	SO4	P	360	-	4,4,4	0.21	0	6,6,6	0.21	0
2	SO4	P	359	-	4,4,4	0.26	0	6,6,6	0.20	0
3	NAD	B	361	-	46,48,48	1.89	9 (19%)	64,73,73	2.25	16 (25%)
2	SO4	O	360	-	4,4,4	0.27	0	6,6,6	0.48	0
2	SO4	Q	360	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	B	360	-	4,4,4	0.25	0	6,6,6	0.20	0
2	SO4	R	360	-	4,4,4	0.28	0	6,6,6	0.24	0
2	SO4	O	359	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	Q	359	-	4,4,4	0.25	0	6,6,6	0.12	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	NAD	A	361	-	-	6/30/62/62	0/5/5/5
3	NAD	Q	361	-	-	12/30/62/62	0/5/5/5
3	NAD	P	361	-	-	11/30/62/62	0/5/5/5
3	NAD	O	361	-	-	17/30/62/62	0/5/5/5
3	NAD	R	361	-	-	14/30/62/62	0/5/5/5
3	NAD	B	361	-	-	10/30/62/62	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	361	NAD	O4D-C1D	6.47	1.49	1.40
3	Q	361	NAD	O4D-C1D	6.33	1.49	1.40
3	Q	361	NAD	C7N-N7N	6.33	1.44	1.33
3	A	361	NAD	C7N-N7N	6.30	1.44	1.33
3	R	361	NAD	C7N-N7N	6.27	1.44	1.33
3	P	361	NAD	C7N-N7N	6.25	1.44	1.33
3	O	361	NAD	C7N-N7N	6.24	1.44	1.33
3	R	361	NAD	O4D-C1D	6.22	1.49	1.40
3	O	361	NAD	O4D-C1D	6.21	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	361	NAD	O4D-C1D	6.18	1.49	1.40
3	B	361	NAD	C7N-N7N	6.11	1.44	1.33
3	P	361	NAD	O4D-C1D	6.05	1.48	1.40
3	O	361	NAD	C6A-N6A	3.79	1.43	1.34
3	Q	361	NAD	C6A-N6A	3.75	1.43	1.34
3	R	361	NAD	C6A-N6A	3.71	1.43	1.34
3	B	361	NAD	C6A-N6A	3.63	1.43	1.34
3	P	361	NAD	C6A-N6A	3.49	1.43	1.34
3	A	361	NAD	C6A-N6A	3.48	1.43	1.34
3	P	361	NAD	O4D-C4D	-3.25	1.37	1.45
3	A	361	NAD	O4D-C4D	-3.12	1.38	1.45
3	O	361	NAD	O4D-C4D	-3.11	1.38	1.45
3	R	361	NAD	O4D-C4D	-3.11	1.38	1.45
3	O	361	NAD	C2B-C3B	-3.09	1.45	1.53
3	R	361	NAD	C2B-C3B	-3.07	1.45	1.53
3	B	361	NAD	O4D-C4D	-3.01	1.38	1.45
3	O	361	NAD	C5A-N7A	-2.93	1.33	1.39
3	Q	361	NAD	O4D-C4D	-2.88	1.38	1.45
3	B	361	NAD	C2B-C3B	-2.82	1.45	1.53
3	B	361	NAD	C5A-N7A	-2.74	1.34	1.39
3	R	361	NAD	C5A-N7A	-2.70	1.34	1.39
3	P	361	NAD	C5A-N7A	-2.65	1.34	1.39
3	Q	361	NAD	C2B-C3B	-2.51	1.46	1.53
3	A	361	NAD	C5A-N7A	-2.47	1.34	1.39
3	O	361	NAD	O3D-C3D	-2.36	1.37	1.43
3	R	361	NAD	O3D-C3D	-2.32	1.37	1.43
3	Q	361	NAD	O3D-C3D	-2.31	1.37	1.43
3	P	361	NAD	O3D-C3D	-2.29	1.37	1.43
3	Q	361	NAD	C5A-N7A	-2.23	1.35	1.39
3	P	361	NAD	C2B-C3B	-2.21	1.47	1.53
3	P	361	NAD	O4B-C4B	-2.16	1.40	1.45
3	B	361	NAD	O3D-C3D	-2.14	1.37	1.43
3	O	361	NAD	O3B-C3B	-2.11	1.37	1.43
3	A	361	NAD	C2B-C3B	-2.10	1.47	1.53
3	R	361	NAD	C2D-C3D	-2.10	1.47	1.53
3	O	361	NAD	O2D-C2D	-2.09	1.37	1.43
3	B	361	NAD	C2D-C3D	-2.07	1.47	1.53
3	O	361	NAD	O2B-C2B	-2.06	1.37	1.43
3	R	361	NAD	C4A-N9A	-2.05	1.33	1.37
3	B	361	NAD	O2D-C2D	-2.04	1.37	1.43
3	A	361	NAD	O2D-C2D	-2.02	1.38	1.43

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	361	NAD	O3-PA-O1A	-11.12	77.25	110.70
3	O	361	NAD	O3-PA-O1A	-10.01	80.59	110.70
3	P	361	NAD	O3-PA-O1A	-9.17	83.10	110.70
3	A	361	NAD	O3-PA-O1A	-9.17	83.10	110.70
3	Q	361	NAD	O3-PA-O1A	-8.57	84.91	110.70
3	B	361	NAD	O3-PA-O1A	-8.40	85.43	110.70
3	B	361	NAD	O2A-PA-O3	-8.14	85.28	107.27
3	P	361	NAD	O2A-PA-O3	-7.99	85.69	107.27
3	O	361	NAD	O2A-PA-O3	-7.07	88.16	107.27
3	A	361	NAD	O2A-PA-O3	-6.52	89.66	107.27
3	R	361	NAD	O2A-PA-O3	-6.51	89.69	107.27
3	Q	361	NAD	O2A-PA-O3	-5.20	93.22	107.27
3	B	361	NAD	C5A-C4A-N3A	-4.73	120.20	126.72
3	Q	361	NAD	C5A-C4A-N3A	-4.62	120.36	126.72
3	O	361	NAD	C5A-C4A-N3A	-4.55	120.45	126.72
3	Q	361	NAD	N9A-C8A-N7A	-4.42	107.66	113.94
3	A	361	NAD	C5A-C4A-N3A	-4.42	120.63	126.72
3	B	361	NAD	N3A-C2A-N1A	-4.40	121.92	128.58
3	R	361	NAD	N3A-C2A-N1A	-4.39	121.94	128.58
3	R	361	NAD	C5A-C4A-N3A	-4.32	120.76	126.72
3	P	361	NAD	N9A-C8A-N7A	-4.32	107.80	113.94
3	O	361	NAD	N3A-C4A-N9A	4.32	134.52	127.17
3	Q	361	NAD	N3A-C2A-N1A	-4.18	122.26	128.58
3	B	361	NAD	N3A-C4A-N9A	4.14	134.20	127.17
3	P	361	NAD	N3A-C2A-N1A	-4.13	122.33	128.58
3	Q	361	NAD	C4A-N9A-C8A	4.05	109.99	105.74
3	O	361	NAD	N3A-C2A-N1A	-4.03	122.48	128.58
3	O	361	NAD	N9A-C8A-N7A	-4.02	108.23	113.94
3	O	361	NAD	C4A-N9A-C8A	4.02	109.96	105.74
3	A	361	NAD	N3A-C2A-N1A	-4.01	122.51	128.58
3	Q	361	NAD	O5B-PA-O1A	3.93	124.50	108.94
3	P	361	NAD	C4A-N9A-C8A	3.93	109.86	105.74
3	Q	361	NAD	N3A-C4A-N9A	3.85	133.72	127.17
3	R	361	NAD	N9A-C8A-N7A	-3.78	108.57	113.94
3	A	361	NAD	N9A-C8A-N7A	-3.76	108.60	113.94
3	A	361	NAD	N3A-C4A-N9A	3.73	133.51	127.17
3	P	361	NAD	C5A-C4A-N3A	-3.65	121.69	126.72
3	Q	361	NAD	C5A-N7A-C8A	3.64	109.17	103.45
3	B	361	NAD	N9A-C8A-N7A	-3.61	108.81	113.94
3	Q	361	NAD	O5D-C5D-C4D	3.44	120.70	108.99
3	B	361	NAD	O5B-C5B-C4B	3.40	120.56	108.99
3	B	361	NAD	C2A-N3A-C4A	3.37	120.06	111.83
3	B	361	NAD	C4A-N9A-C8A	3.34	109.24	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	361	NAD	C2A-N3A-C4A	3.32	119.94	111.83
3	A	361	NAD	C4A-N9A-C8A	3.30	109.20	105.74
3	R	361	NAD	O5B-PA-O1A	3.29	121.98	108.94
3	Q	361	NAD	C2A-N3A-C4A	3.27	119.81	111.83
3	P	361	NAD	C5A-N7A-C8A	3.16	108.42	103.45
3	R	361	NAD	C3N-C7N-N7N	3.14	121.60	117.74
3	A	361	NAD	C2A-N3A-C4A	3.13	119.48	111.83
3	R	361	NAD	C4A-N9A-C8A	3.11	109.00	105.74
3	O	361	NAD	C2A-N3A-C4A	3.09	119.39	111.83
3	R	361	NAD	N3A-C4A-N9A	3.08	132.41	127.17
3	R	361	NAD	O5B-C5B-C4B	3.06	119.40	108.99
3	B	361	NAD	O5B-PA-O1A	3.02	120.92	108.94
3	P	361	NAD	N3A-C4A-N9A	3.02	132.31	127.17
3	O	361	NAD	O5B-C5B-C4B	3.01	119.26	108.99
3	A	361	NAD	O5B-PA-O1A	2.99	120.78	108.94
3	O	361	NAD	C5A-N7A-C8A	2.98	108.14	103.45
3	Q	361	NAD	C4A-C5A-N7A	-2.98	107.17	110.58
3	B	361	NAD	C5A-N7A-C8A	2.95	108.09	103.45
3	R	361	NAD	O5D-C5D-C4D	2.95	119.02	108.99
3	R	361	NAD	C5A-N7A-C8A	2.91	108.03	103.45
3	O	361	NAD	O4B-C1B-N9A	2.86	113.59	108.09
3	B	361	NAD	O2A-PA-O5B	2.86	120.52	107.57
3	P	361	NAD	C2A-N3A-C4A	2.84	118.77	111.83
3	A	361	NAD	C5A-N7A-C8A	2.84	107.91	103.45
3	P	361	NAD	O5D-C5D-C4D	2.83	118.64	108.99
3	O	361	NAD	O5B-PA-O1A	2.83	120.16	108.94
3	B	361	NAD	C3N-C7N-N7N	2.76	121.14	117.74
3	P	361	NAD	O5B-C5B-C4B	2.66	118.06	108.99
3	R	361	NAD	C4A-C5A-N7A	-2.65	107.56	110.58
3	P	361	NAD	O5B-PA-O1A	2.62	119.31	108.94
3	P	361	NAD	C3N-C7N-N7N	2.62	120.96	117.74
3	P	361	NAD	C4B-O4B-C1B	-2.57	103.78	109.47
3	P	361	NAD	C4A-C5A-N7A	-2.49	107.73	110.58
3	P	361	NAD	C4A-N9A-C1B	-2.47	120.86	126.63
3	P	361	NAD	C2D-C3D-C4D	2.45	107.35	102.61
3	R	361	NAD	O4B-C1B-N9A	2.43	112.76	108.09
3	B	361	NAD	O5D-C5D-C4D	2.39	117.13	108.99
3	O	361	NAD	O2A-PA-O5B	2.36	118.25	107.57
3	O	361	NAD	C5A-C6A-N6A	-2.34	117.49	123.29
3	A	361	NAD	O5B-C5B-C4B	2.31	116.86	108.99
3	A	361	NAD	C2D-C3D-C4D	2.28	107.02	102.61
3	P	361	NAD	O2A-PA-O5B	2.27	117.88	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	361	NAD	O2A-PA-O5B	2.26	117.79	107.57
3	O	361	NAD	C2D-C3D-C4D	2.25	106.95	102.61
3	A	361	NAD	O7N-C7N-N7N	-2.22	119.41	122.62
3	O	361	NAD	C5N-C4N-C3N	-2.09	118.31	120.36
3	B	361	NAD	C2D-C3D-C4D	2.09	106.64	102.61
3	P	361	NAD	O7N-C7N-N7N	-2.08	119.61	122.62
3	B	361	NAD	C4A-C5A-N7A	-2.08	108.20	110.58
3	R	361	NAD	O2A-PA-O1A	2.05	122.00	112.44
3	O	361	NAD	C4D-O4D-C1D	-2.02	108.08	109.92
3	A	361	NAD	C4A-C5A-N7A	-2.02	108.28	110.58

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	361	NAD	C5B-O5B-PA-O3
3	A	361	NAD	O4D-C1D-N1N-C2N
3	A	361	NAD	O4D-C1D-N1N-C6N
3	B	361	NAD	C5B-O5B-PA-O3
3	B	361	NAD	O4D-C1D-N1N-C2N
3	B	361	NAD	O4D-C1D-N1N-C6N
3	B	361	NAD	C2N-C3N-C7N-O7N
3	B	361	NAD	C2N-C3N-C7N-N7N
3	O	361	NAD	C5B-O5B-PA-O3
3	O	361	NAD	C5D-O5D-PN-O3
3	O	361	NAD	C5D-O5D-PN-O1N
3	O	361	NAD	C5D-O5D-PN-O2N
3	O	361	NAD	O4D-C1D-N1N-C2N
3	O	361	NAD	O4D-C1D-N1N-C6N
3	P	361	NAD	C5B-O5B-PA-O1A
3	P	361	NAD	O4D-C1D-N1N-C2N
3	P	361	NAD	O4D-C1D-N1N-C6N
3	P	361	NAD	C2D-C1D-N1N-C6N
3	Q	361	NAD	C5B-O5B-PA-O3
3	Q	361	NAD	C5D-O5D-PN-O2N
3	Q	361	NAD	O4D-C1D-N1N-C2N
3	Q	361	NAD	O4D-C1D-N1N-C6N
3	R	361	NAD	C5B-O5B-PA-O3
3	R	361	NAD	O4D-C1D-N1N-C2N
3	B	361	NAD	C4N-C3N-C7N-N7N
3	B	361	NAD	C4N-C3N-C7N-O7N
3	O	361	NAD	C4N-C3N-C7N-O7N

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Mol	Chain	Res	Type	Atoms
3	O	361	NAD	C2N-C3N-C7N-O7N
3	Q	361	NAD	C2N-C3N-C7N-O7N
3	Q	361	NAD	C2N-C3N-C7N-N7N
3	R	361	NAD	C2N-C3N-C7N-O7N
3	R	361	NAD	C2N-C3N-C7N-N7N
3	Q	361	NAD	C4N-C3N-C7N-O7N
3	Q	361	NAD	C4N-C3N-C7N-N7N
3	R	361	NAD	O4B-C4B-C5B-O5B
3	R	361	NAD	C3B-C4B-C5B-O5B
3	R	361	NAD	C4N-C3N-C7N-N7N
3	R	361	NAD	C4N-C3N-C7N-O7N
3	B	361	NAD	O4B-C4B-C5B-O5B
3	P	361	NAD	C2N-C3N-C7N-N7N
3	B	361	NAD	C3B-C4B-C5B-O5B
3	P	361	NAD	C4N-C3N-C7N-N7N
3	O	361	NAD	O4B-C4B-C5B-O5B
3	Q	361	NAD	O4B-C4B-C5B-O5B
3	Q	361	NAD	C3B-C4B-C5B-O5B
3	O	361	NAD	C4N-C3N-C7N-N7N
3	O	361	NAD	C3B-C4B-C5B-O5B
3	O	361	NAD	C2N-C3N-C7N-N7N
3	A	361	NAD	O4B-C4B-C5B-O5B
3	B	361	NAD	PN-O3-PA-O1A
3	O	361	NAD	C4B-C5B-O5B-PA
3	O	361	NAD	PN-O3-PA-O5B
3	A	361	NAD	C3B-C4B-C5B-O5B
3	P	361	NAD	C4N-C3N-C7N-O7N
3	A	361	NAD	PN-O3-PA-O2A
3	O	361	NAD	PA-O3-PN-O2N
3	P	361	NAD	C2N-C3N-C7N-O7N
3	O	361	NAD	C5B-O5B-PA-O2A
3	Q	361	NAD	C5D-O5D-PN-O3
3	Q	361	NAD	C5D-O5D-PN-O1N
3	R	361	NAD	C5B-O5B-PA-O2A
3	P	361	NAD	PN-O3-PA-O2A
3	R	361	NAD	PN-O3-PA-O1A
3	P	361	NAD	C2D-C1D-N1N-C2N
3	R	361	NAD	O4D-C4D-C5D-O5D
3	R	361	NAD	O4D-C1D-N1N-C6N
3	R	361	NAD	C4B-C5B-O5B-PA
3	R	361	NAD	C2B-C1B-N9A-C8A
3	O	361	NAD	PA-O3-PN-O1N

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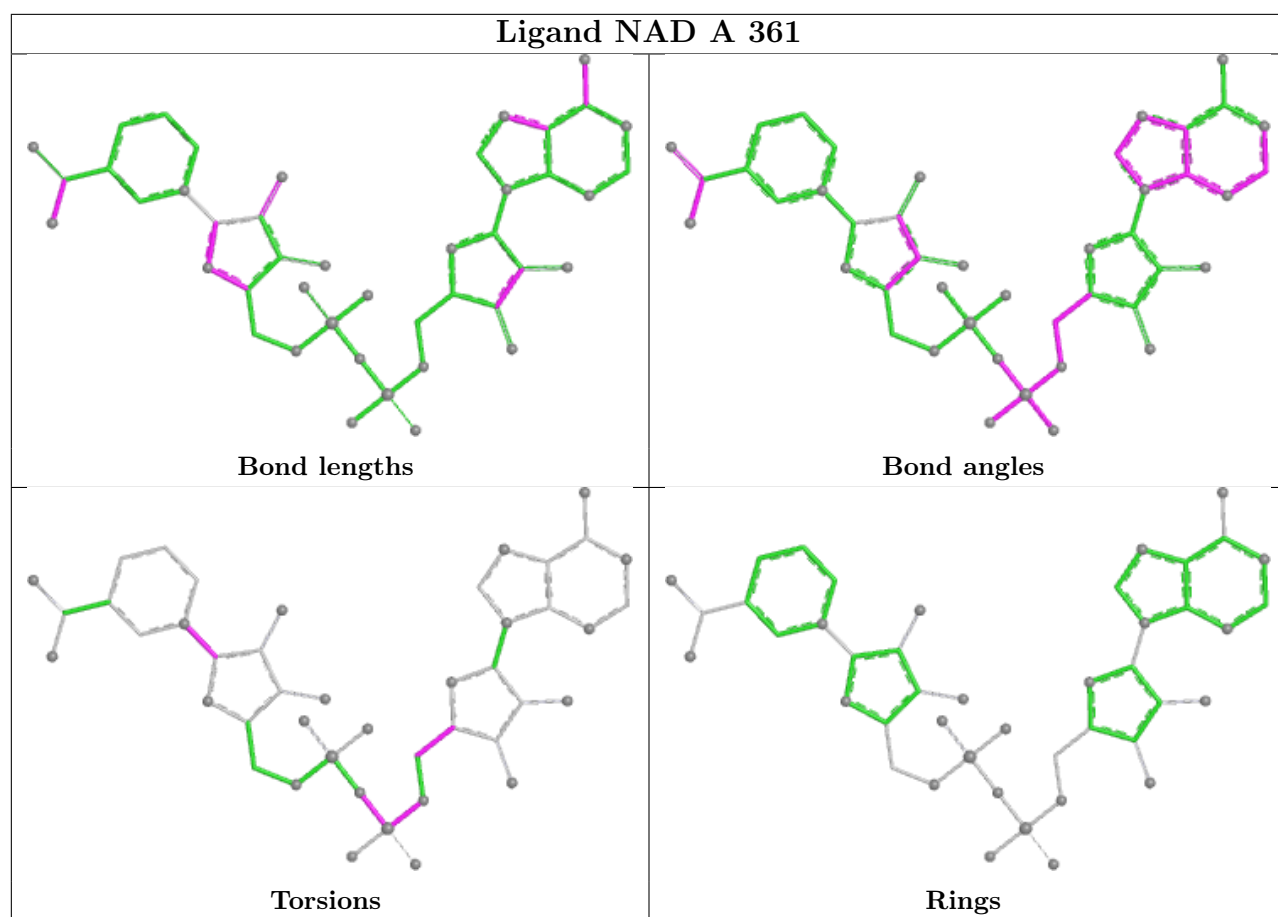
Mol	Chain	Res	Type	Atoms
3	P	361	NAD	PN-O3-PA-O1A

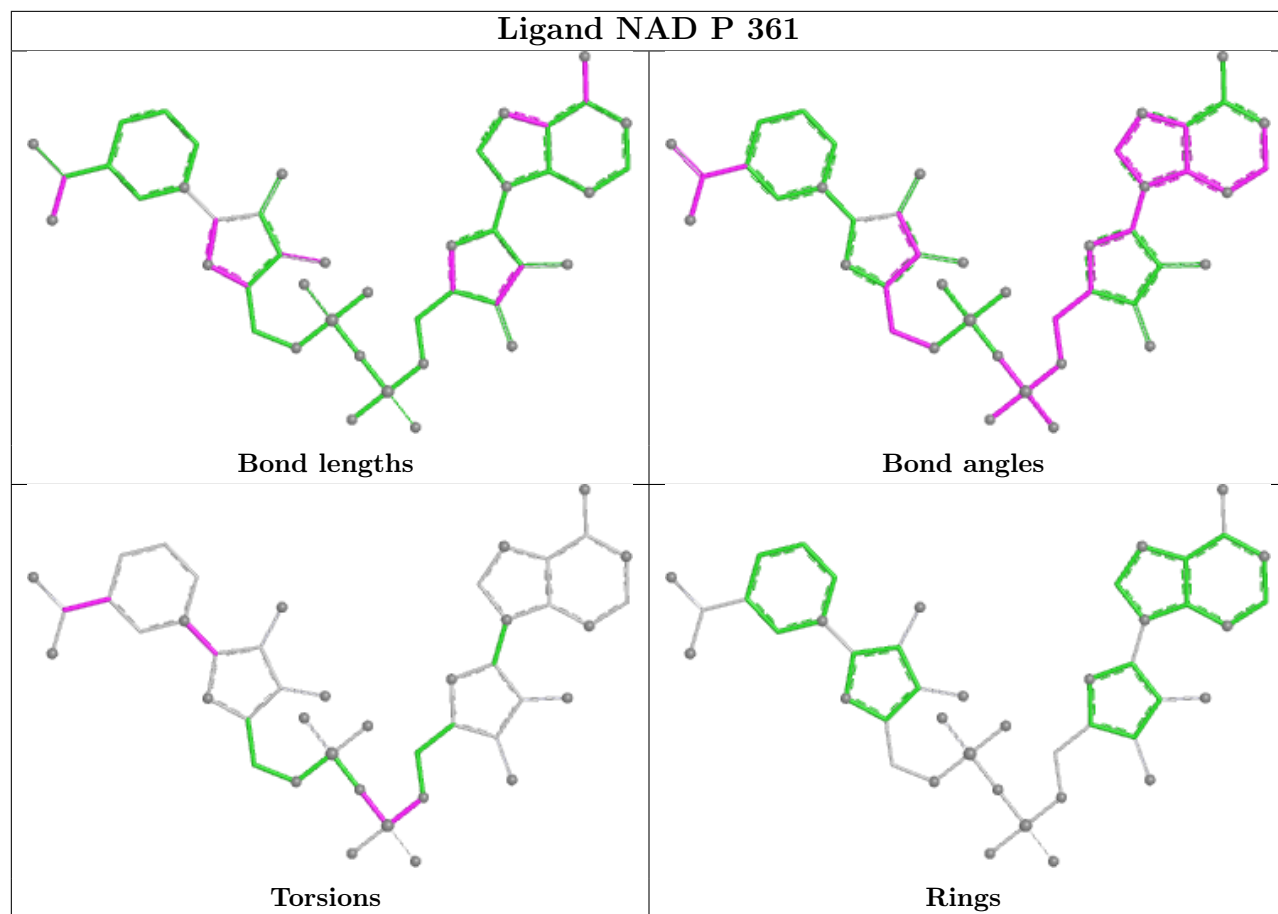
There are no ring outliers.

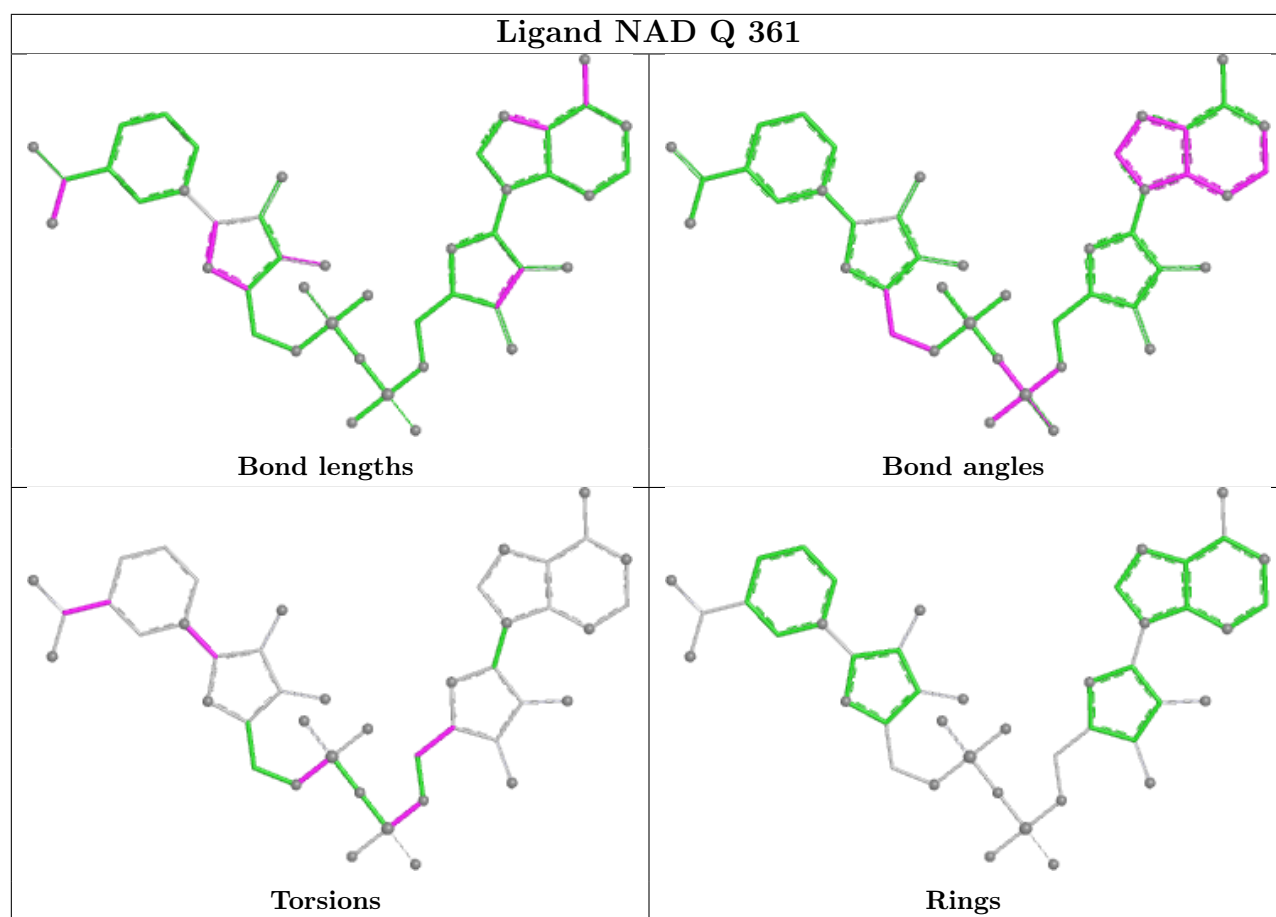
9 monomers are involved in 23 short contacts:

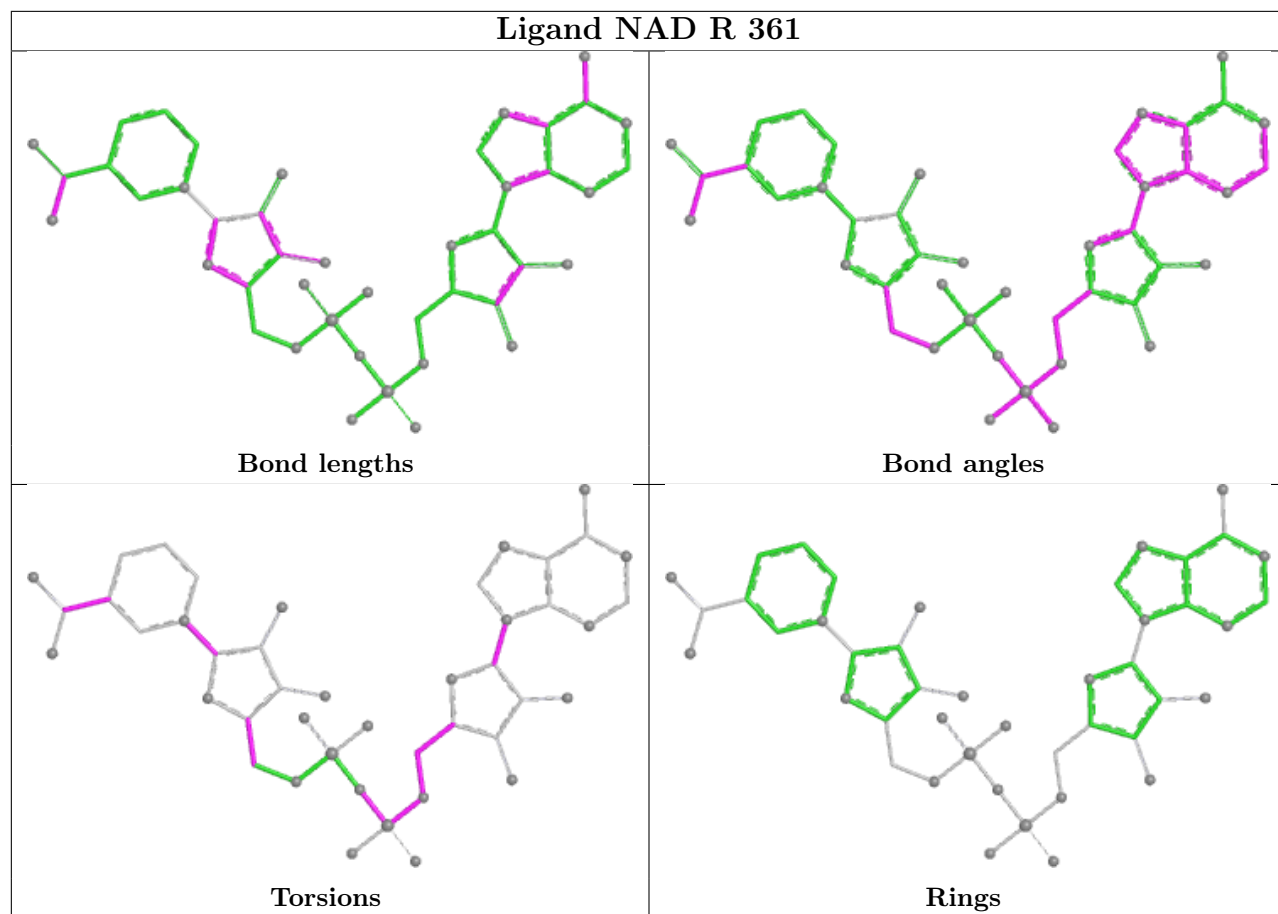
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	361	NAD	2	0
3	P	361	NAD	3	0
3	Q	361	NAD	6	0
3	R	361	NAD	3	0
3	O	361	NAD	3	0
2	P	360	SO4	1	0
3	B	361	NAD	3	0
2	B	360	SO4	1	0
2	R	360	SO4	1	0

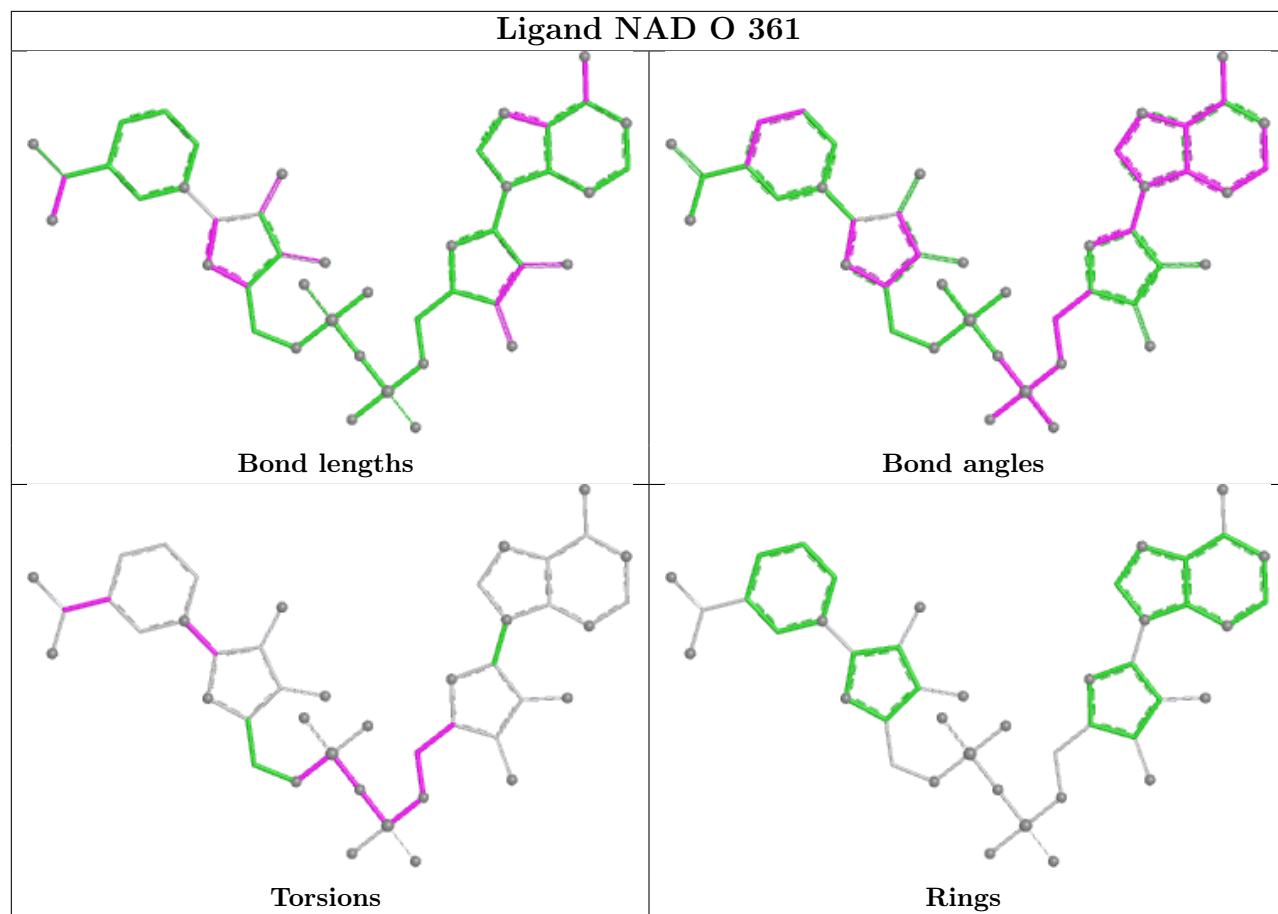
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

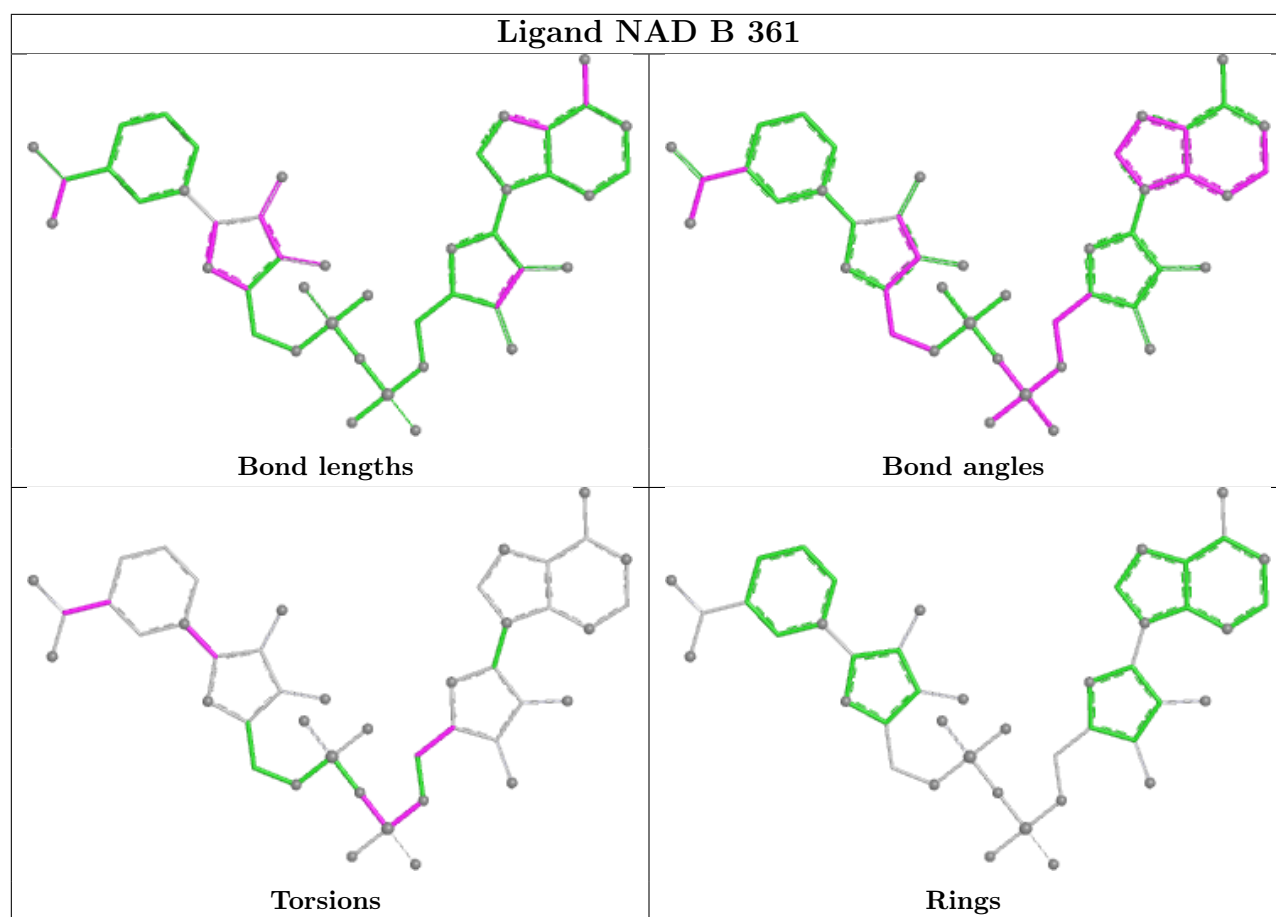












5.7 Other polymers [i](#)

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 [i](#)

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

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	358/359 (99%)	-1.10	0 100 100	3, 26, 78, 196	0
1	B	358/359 (99%)	-1.07	0 100 100	4, 28, 74, 188	0
1	O	358/359 (99%)	-1.05	0 100 100	6, 27, 72, 187	0
1	P	358/359 (99%)	-1.05	1 (0%) 90 81	4, 26, 76, 188	0
1	Q	358/359 (99%)	-1.03	0 100 100	9, 29, 77, 188	0
1	R	358/359 (99%)	-1.10	0 100 100	5, 27, 76, 190	0
All	All	2148/2154 (99%)	-1.07	1 (0%) 100 100	3, 27, 76, 196	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	355	ALA	2.1

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](#)

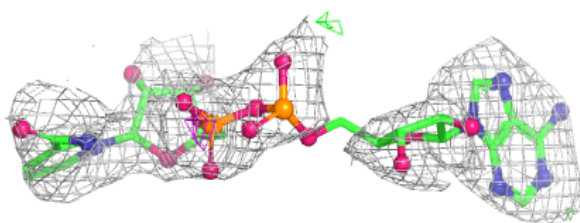
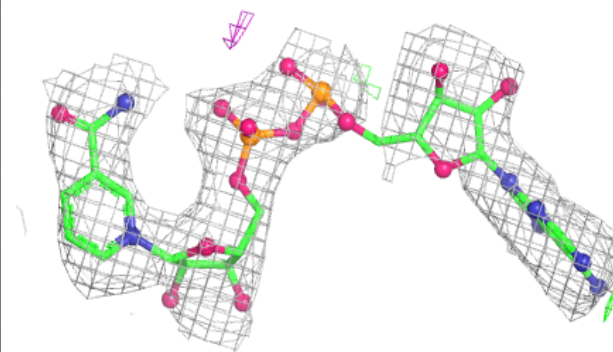
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	SO4	P	360	5/5	0.85	0.11	116,118,121,121	0
2	SO4	B	359	5/5	0.92	0.09	99,103,105,108	0
2	SO4	P	359	5/5	0.93	0.06	79,84,85,87	0
2	SO4	R	359	5/5	0.94	0.07	79,86,86,88	0
2	SO4	R	360	5/5	0.94	0.07	83,86,89,90	0
2	SO4	A	360	5/5	0.95	0.07	86,92,92,93	0
2	SO4	Q	359	5/5	0.96	0.07	102,104,105,106	0
2	SO4	Q	360	5/5	0.96	0.07	95,95,97,99	0
2	SO4	A	359	5/5	0.96	0.07	81,84,88,92	0
2	SO4	B	360	5/5	0.96	0.07	106,108,110,111	0
2	SO4	O	359	5/5	0.97	0.05	95,99,101,102	0
3	NAD	A	361	44/44	0.97	0.06	4,43,57,155	0
3	NAD	P	361	44/44	0.97	0.06	5,42,54,194	0
3	NAD	Q	361	44/44	0.97	0.06	0,44,63,202	0
3	NAD	R	361	44/44	0.97	0.06	0,37,49,124	0
2	SO4	O	360	5/5	0.98	0.08	96,97,98,100	0
3	NAD	B	361	44/44	0.98	0.06	16,48,74,138	0
3	NAD	O	361	44/44	0.98	0.05	0,47,63,155	0

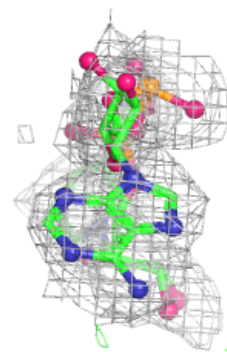
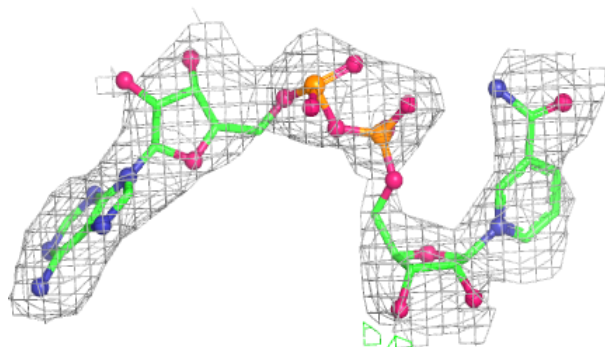
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 361:

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

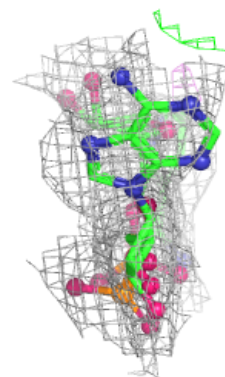
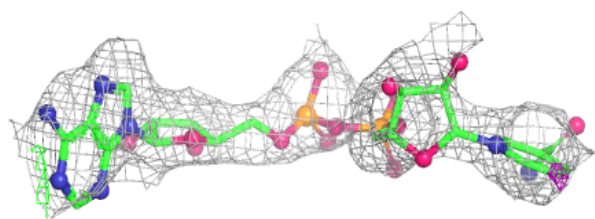
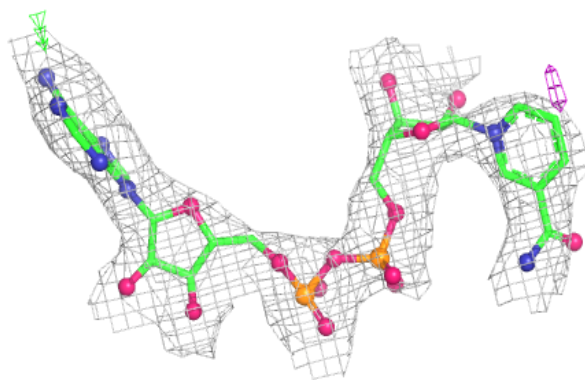
**Electron density around NAD P 361:**

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

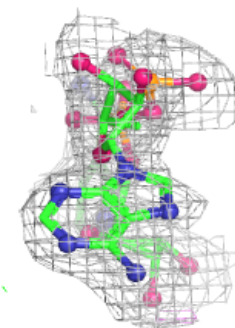
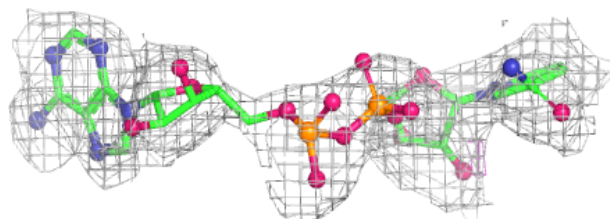
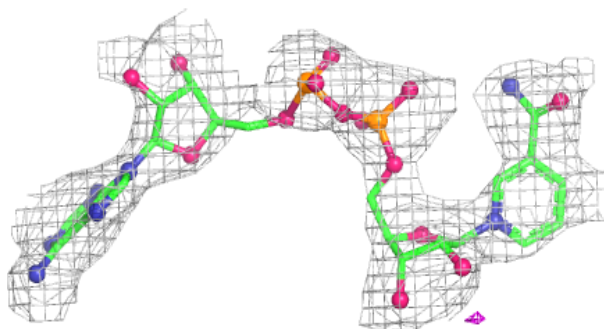


Electron density around NAD Q 361:

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

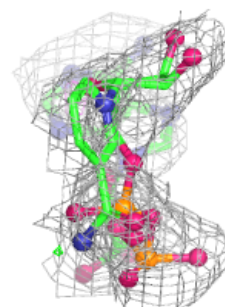
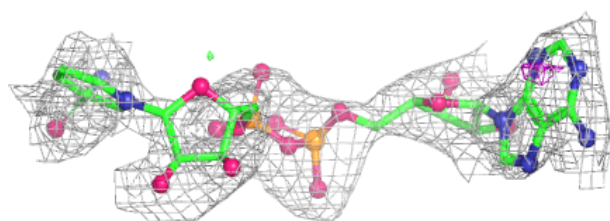
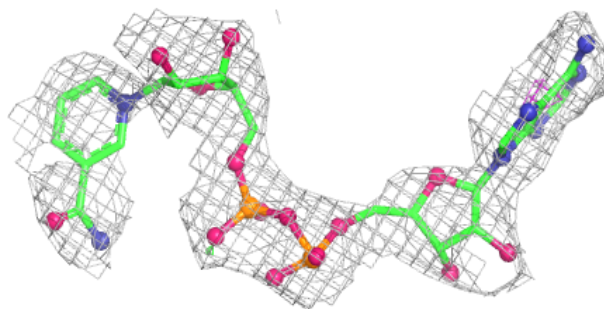
**Electron density around NAD R 361:**

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

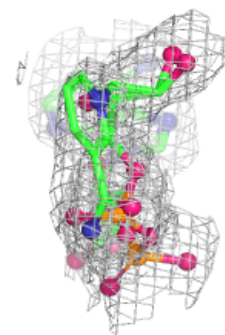
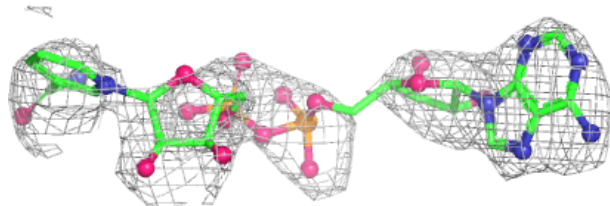
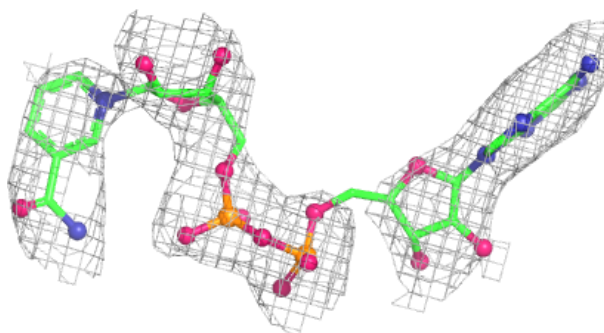


Electron density around NAD B 361:

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

**Electron density around NAD O 361:**

$2mF_o-DF_c$ (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.