



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:52 AM UTC

PDB ID : 1NFB / pdb_00001nfb
Title : Ternary complex of the human type II Inosine Monophosphate Dedhydrogenase with 6Cl-IMP and NAD
Authors : Risal, D.; Strickler, M.D.; Goldstein, B.M.
Deposited on : 2002-12-13
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

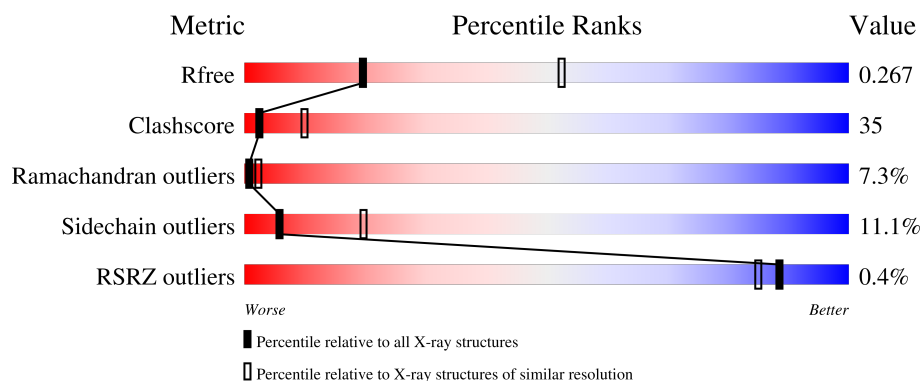
1 Overall quality at a glance

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	514	
1	B	514	

2 Entry composition [i](#)

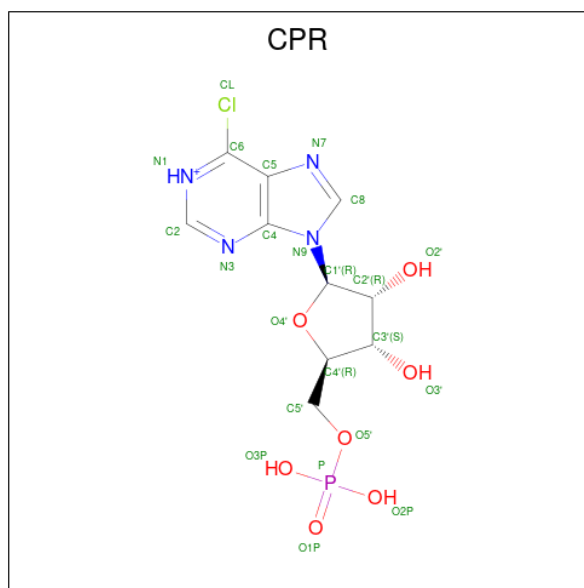
There are 4 unique types of molecules in this entry. The entry contains 5885 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Inosine-5'-monophosphate dehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			2833	1783	489	545	16			
1	B	396	Total	C	N	O	S	0	0	0
			2833	1783	489	545	16			

- Molecule 2 is 6-CHLOROPURINE RIBOSIDE, 5'-MONOPHOSPHATE (CCD ID: CPR) (formula: $C_{10}H_{13}ClN_4O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	4	7	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

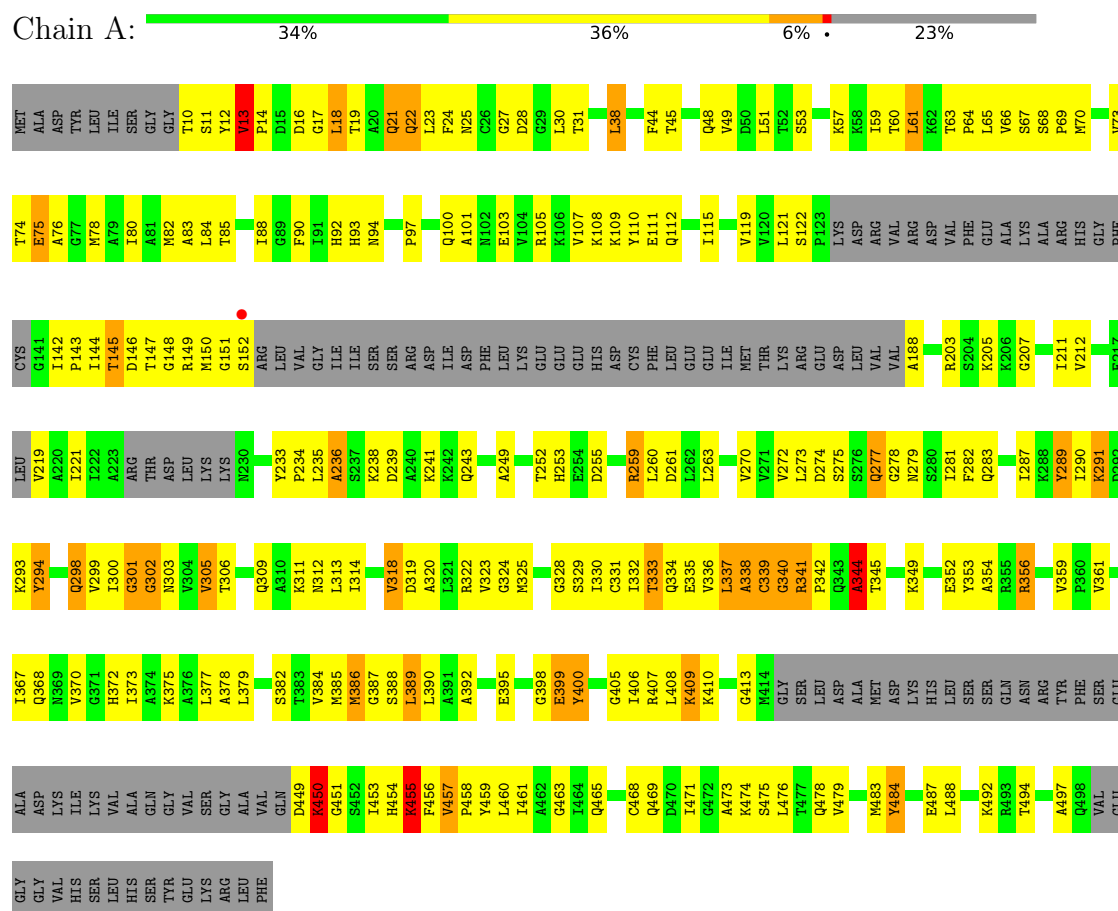
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	43	Total O 43 43	0	0
4	B	44	Total O 44 44	0	0

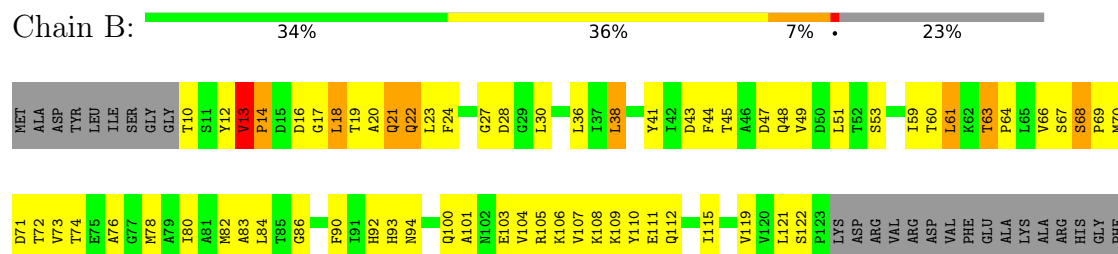
3 Residue-property plots

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: Inosine-5'-monophosphate dehydrogenase 2



• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	145.19Å 145.19Å 127.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.82 – 2.90 47.82 – 2.90	Depositor EDS
% Data completeness (in resolution range)	66.5 (47.82-2.90) 74.6 (47.82-2.90)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.274 0.245 , 0.267	Depositor DCC
R_{free} test set	2455 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 91.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.447 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5885	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: CPR, 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	0.61	1/2870 (0.0%)	1.14	26/3881 (0.7%)
1	B	0.62	1/2870 (0.0%)	1.14	22/3881 (0.6%)
All	All	0.62	2/5740 (0.0%)	1.14	48/7762 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	457	VAL	CA-CB	-6.77	1.50	1.54
1	A	457	VAL	CA-CB	-6.59	1.50	1.54

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406	ILE	N-CA-C	10.82	122.02	108.82
1	A	406	ILE	N-CA-C	10.70	121.88	108.82
1	B	68	SER	N-CA-C	8.28	120.34	109.83
1	A	398	GLY	N-CA-C	7.93	121.34	110.56
1	B	398	GLY	N-CA-C	7.92	121.33	110.56
1	A	142	ILE	N-CA-C	7.76	117.20	108.05
1	A	38	LEU	CA-C-N	7.74	127.69	120.03
1	A	38	LEU	C-N-CA	7.74	127.69	120.03
1	B	142	ILE	N-CA-C	7.71	117.15	108.05
1	A	68	SER	N-CA-C	7.43	120.34	110.08
1	B	38	LEU	CA-C-N	7.16	127.12	120.03
1	B	38	LEU	C-N-CA	7.16	127.12	120.03
1	B	333	THR	CB-CA-C	-7.15	108.34	116.63
1	A	333	THR	CB-CA-C	-6.96	108.56	116.63
1	B	301	GLY	N-CA-C	6.84	120.97	112.14
1	A	301	GLY	N-CA-C	6.74	120.83	112.14
1	A	407	ARG	N-CA-C	6.35	119.49	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	407	ARG	N-CA-C	6.32	119.45	109.96
1	A	450	LYS	N-CA-C	6.01	123.61	110.80
1	A	450	LYS	CB-CG-CD	5.98	125.05	111.30
1	B	119	VAL	N-CA-C	5.93	115.87	106.32
1	A	413	GLY	N-CA-C	5.88	119.69	111.10
1	A	119	VAL	N-CA-C	5.85	115.75	106.32
1	B	413	GLY	N-CA-C	5.81	119.59	111.10
1	A	143	PRO	N-CA-C	-5.79	100.55	112.47
1	B	455	LYS	N-CA-C	-5.75	105.28	112.93
1	A	484	TYR	N-CA-C	-5.74	105.54	112.54
1	B	143	PRO	N-CA-C	-5.74	100.65	112.47
1	A	13	VAL	CA-C-N	5.67	126.92	119.84
1	A	13	VAL	C-N-CA	5.67	126.92	119.84
1	B	74	THR	N-CA-C	5.66	118.19	109.07
1	B	450	LYS	N-CA-C	5.54	122.60	110.80
1	B	457	VAL	CB-CA-C	-5.49	108.49	113.70
1	A	455	LYS	N-CA-C	-5.48	105.65	112.93
1	A	74	THR	N-CA-C	5.45	117.85	109.07
1	B	495	SER	N-CA-C	-5.42	104.41	111.02
1	A	121	LEU	N-CA-C	5.37	116.68	107.28
1	B	121	LEU	N-CA-C	5.36	116.66	107.28
1	A	341	ARG	N-CA-C	5.35	121.63	109.81
1	B	484	TYR	N-CA-C	-5.34	106.03	112.54
1	B	341	ARG	N-CA-C	5.30	121.53	109.81
1	A	341	ARG	CA-C-N	5.29	125.54	119.83
1	A	341	ARG	C-N-CA	5.29	125.54	119.83
1	A	294	TYR	CA-C-N	5.05	124.77	119.82
1	A	294	TYR	C-N-CA	5.05	124.77	119.82
1	B	345	THR	N-CA-C	-5.04	105.97	111.82
1	B	364	ASP	N-CA-C	5.04	116.52	108.41
1	A	344	ALA	N-CA-C	-5.01	100.13	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2833	0	2702	197	0
1	B	2833	0	2702	192	0
2	A	22	0	11	2	0
2	B	22	0	11	3	0
3	A	44	0	26	4	0
3	B	44	0	26	5	0
4	A	43	0	0	8	0
4	B	44	0	0	6	0
All	All	5885	0	5478	393	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 35.

All (393) 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:270:VAL:HG12	1:B:298:GLN:HB2	1.30	1.10
1:B:334:GLN:HB3	1:B:337:LEU:HB3	1.42	1.02
1:A:270:VAL:HG12	1:A:298:GLN:HB2	1.43	1.00
1:B:305:VAL:H	1:B:309:GLN:NE2	1.61	0.97
1:A:28:ASP:HB3	1:A:30:LEU:HG	1.48	0.94
1:A:332:ILE:HG12	1:A:333:THR:H	1.33	0.93
1:B:67:SER:HB3	1:B:82:MET:HE3	1.50	0.92
1:B:28:ASP:HB3	1:B:30:LEU:HG	1.54	0.90
1:B:332:ILE:HG12	1:B:333:THR:H	1.39	0.87
1:A:67:SER:HB3	1:A:82:MET:HE3	1.57	0.87
1:A:45:THR:H	1:A:48:GLN:NE2	1.76	0.84
1:B:305:VAL:H	1:B:309:GLN:HE22	1.28	0.82
1:A:303:ASN:OD1	1:A:322:ARG:HD3	1.78	0.81
1:B:473:ALA:HA	1:B:478:GLN:HE21	1.45	0.81
1:B:486:GLY:O	1:B:489:LYS:HE2	1.80	0.80
1:B:386:MET:HE3	1:B:389:LEU:HD23	1.62	0.80
1:A:298:GLN:HE21	1:A:298:GLN:HA	1.47	0.80
1:A:45:THR:H	1:A:48:GLN:HE21	1.27	0.79
1:A:105:ARG:HH12	1:A:109:LYS:HE3	1.48	0.78
1:B:291:LYS:HA	1:B:291:LYS:NZ	1.98	0.77
1:B:92:HIS:HD2	1:B:94:ASN:H	1.33	0.76
1:A:337:LEU:HD12	1:A:339:CYS:H	1.49	0.76
1:B:291:LYS:HA	1:B:291:LYS:HZ1	1.51	0.76
1:A:252:THR:HG21	1:A:283:GLN:HG2	1.68	0.75
1:B:303:ASN:OD1	1:B:322:ARG:HD3	1.87	0.74
1:B:483:MET:HE3	1:B:484:TYR:CE2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:HIS:HA	3:B:702:NAD:H61A	1.53	0.74
1:B:257:LYS:HG2	1:B:289:TYR:CE2	2.23	0.73
1:A:253:HIS:HA	3:A:701:NAD:H61A	1.51	0.73
3:A:701:NAD:O3	3:A:701:NAD:H3D	1.89	0.73
3:B:702:NAD:O3	3:B:702:NAD:H3D	1.89	0.72
1:A:253:HIS:HA	3:A:701:NAD:N6A	2.04	0.72
1:A:92:HIS:CD2	1:A:94:ASN:H	2.08	0.71
1:B:253:HIS:HA	3:B:702:NAD:N6A	2.05	0.71
1:B:330:ILE:HG23	1:B:335:GLU:HB2	1.71	0.71
1:A:330:ILE:HG23	1:A:335:GLU:HB2	1.72	0.71
1:A:334:GLN:HB2	1:A:337:LEU:HB3	1.71	0.71
1:A:277:GLN:CA	1:A:277:GLN:HE21	2.04	0.70
1:B:105:ARG:HH12	1:B:109:LYS:HG2	1.57	0.70
1:B:305:VAL:N	1:B:309:GLN:HE22	1.90	0.70
1:A:291:LYS:NZ	1:A:291:LYS:HA	2.07	0.69
1:A:483:MET:HB3	1:A:488:LEU:HD23	1.74	0.69
1:A:105:ARG:HH22	1:A:109:LYS:HE3	1.56	0.69
1:B:232:ASP:OD1	1:B:234:PRO:HD3	1.93	0.68
1:B:241:LYS:O	1:B:243:GLN:HG3	1.94	0.67
1:A:84:LEU:HB3	1:A:233:TYR:CD2	2.29	0.67
1:B:305:VAL:N	1:B:309:GLN:NE2	2.41	0.67
1:B:300:ILE:HG12	1:B:320:ALA:HB3	1.76	0.67
1:A:334:GLN:CB	1:A:337:LEU:HB3	2.25	0.66
1:A:311:LYS:HD3	4:A:709:HOH:O	1.97	0.65
1:B:257:LYS:HG2	1:B:289:TYR:HE2	1.61	0.65
1:B:386:MET:CE	1:B:389:LEU:HD23	2.26	0.65
1:B:66:VAL:O	1:B:385:MET:HA	1.96	0.65
1:B:84:LEU:HB3	1:B:233:TYR:CD2	2.31	0.65
1:A:28:ASP:HB2	4:A:705:HOH:O	1.95	0.65
1:B:270:VAL:CG1	1:B:298:GLN:HB2	2.18	0.65
1:A:57:LYS:HE3	1:A:319:ASP:HA	1.79	0.65
1:A:19:THR:HB	1:A:22:GLN:HG2	1.80	0.64
1:A:69:PRO:HG3	1:A:90:PHE:HB3	1.79	0.64
1:A:306:THR:OG1	1:A:309:GLN:HG3	1.98	0.64
1:A:66:VAL:O	1:A:385:MET:HA	1.98	0.64
1:A:30:LEU:O	1:A:344:ALA:HB3	1.97	0.63
1:A:293:LYS:HG2	1:A:294:TYR:CE2	2.33	0.63
1:B:337:LEU:HD12	1:B:339:CYS:H	1.62	0.63
1:A:298:GLN:HA	1:A:298:GLN:NE2	2.14	0.63
1:A:323:VAL:HG23	1:A:361:VAL:HG13	1.80	0.63
1:B:70:MET:SD	2:B:631:CPR:H8	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:SER:O	1:B:303:ASN:HB2	1.99	0.63
1:A:270:VAL:CG1	1:A:298:GLN:HB2	2.26	0.63
3:B:702:NAD:H3D	3:B:702:NAD:PN	2.39	0.62
1:B:314:ILE:HA	1:B:318:VAL:HG22	1.81	0.62
1:A:377:LEU:HD13	1:A:476:LEU:HD13	1.82	0.62
1:A:473:ALA:HA	1:A:478:GLN:HE21	1.65	0.62
1:B:36:LEU:HG	1:B:493:ARG:NH1	2.14	0.62
1:A:188:ALA:HB3	1:A:211:ILE:HA	1.82	0.61
1:A:61:LEU:N	1:A:61:LEU:HD23	2.15	0.61
1:A:241:LYS:O	1:A:243:GLN:HG3	1.99	0.61
1:A:275:SER:O	1:A:303:ASN:HB2	2.01	0.61
1:A:332:ILE:CG1	1:A:333:THR:H	2.11	0.61
1:A:73:VAL:HG11	1:A:387:GLY:HA2	1.81	0.61
1:B:395:GLU:OE1	1:B:453:ILE:HG12	2.00	0.61
1:A:59:ILE:CD1	1:A:270:VAL:HG13	2.30	0.61
3:A:701:NAD:H3D	3:A:701:NAD:PN	2.40	0.61
1:A:59:ILE:HD12	1:A:270:VAL:HG13	1.82	0.61
1:B:30:LEU:O	1:B:344:ALA:HB3	2.01	0.61
1:A:277:GLN:HE21	1:A:277:GLN:C	2.09	0.60
1:B:303:ASN:ND2	1:B:324:GLY:O	2.34	0.60
1:B:69:PRO:HG3	1:B:90:PHE:HB3	1.84	0.60
1:B:76:ALA:O	1:B:80:ILE:HG13	2.02	0.60
1:B:45:THR:H	1:B:48:GLN:NE2	2.00	0.60
1:B:78:MET:SD	1:B:82:MET:HE2	2.42	0.60
1:A:66:VAL:HG13	1:A:88:ILE:HG23	1.84	0.60
1:A:59:ILE:HD12	1:A:270:VAL:CG1	2.32	0.60
1:A:105:ARG:NH1	1:A:109:LYS:HE3	2.16	0.60
1:B:370:VAL:HG11	1:B:463:GLY:HA3	1.84	0.59
1:A:328:GLY:HA2	4:A:744:HOH:O	2.02	0.59
1:A:332:ILE:HG12	1:A:333:THR:N	2.10	0.59
1:B:188:ALA:CB	1:B:211:ILE:HA	2.32	0.59
1:B:188:ALA:HB3	1:B:211:ILE:HA	1.83	0.59
1:A:494:THR:OG1	1:A:497:ALA:HB2	2.02	0.59
1:B:245:LEU:HD11	4:B:705:HOH:O	2.02	0.59
1:B:461:ILE:O	1:B:465:GLN:HG3	2.03	0.59
1:B:23:LEU:O	1:B:23:LEU:HD12	2.03	0.59
1:A:314:ILE:HA	1:A:318:VAL:HG22	1.84	0.58
1:B:483:MET:HB3	1:B:488:LEU:HD23	1.85	0.58
1:A:303:ASN:ND2	1:A:324:GLY:O	2.36	0.58
1:B:325:MET:HG2	1:B:340:GLY:HA2	1.86	0.58
1:A:75:GLU:HG2	4:A:741:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:HIS:CD2	1:B:94:ASN:H	2.18	0.58
1:A:188:ALA:CB	1:A:211:ILE:HA	2.34	0.57
1:B:36:LEU:HD12	1:B:493:ARG:HD3	1.86	0.57
1:A:28:ASP:HB3	1:A:30:LEU:CG	2.27	0.57
1:A:69:PRO:HG3	1:A:90:PHE:CB	2.35	0.57
1:A:333:THR:HG22	1:A:334:GLN:N	2.19	0.57
1:A:330:ILE:HG12	1:A:335:GLU:HG2	1.86	0.57
1:B:252:THR:HA	1:B:286:MET:HE3	1.85	0.57
1:A:78:MET:SD	1:A:82:MET:HE2	2.45	0.57
1:B:252:THR:HG21	1:B:283:GLN:HG2	1.86	0.57
1:B:242:LYS:HD2	1:B:242:LYS:N	2.20	0.56
1:B:273:LEU:CB	1:B:283:GLN:HE22	2.17	0.56
1:B:452:SER:HB3	1:B:455:LYS:HE3	1.86	0.56
1:A:300:ILE:HG12	1:A:320:ALA:HB3	1.87	0.56
1:B:69:PRO:HG3	1:B:90:PHE:CB	2.36	0.56
1:B:71:ASP:HA	1:B:92:HIS:ND1	2.20	0.56
1:B:12:TYR:O	1:B:13:VAL:HG22	2.05	0.56
1:B:333:THR:HG22	1:B:334:GLN:N	2.20	0.56
1:A:313:LEU:O	1:A:318:VAL:HG22	2.05	0.56
1:B:71:ASP:HA	1:B:92:HIS:CE1	2.41	0.56
1:B:453:ILE:HG23	1:B:457:VAL:HG23	1.87	0.56
1:B:10:THR:HG22	1:B:12:TYR:H	1.70	0.55
1:A:298:GLN:HE21	1:A:298:GLN:CA	2.18	0.55
1:A:392:ALA:HB1	1:A:449:ASP:OD2	2.07	0.55
1:B:378:ALA:O	1:B:483:MET:HG2	2.05	0.55
1:A:333:THR:HG22	1:A:334:GLN:H	1.71	0.55
1:A:370:VAL:HG11	1:A:463:GLY:HA3	1.89	0.55
1:A:386:MET:HE1	1:A:460:LEU:HD11	1.87	0.55
1:B:483:MET:HE3	1:B:484:TYR:CZ	2.42	0.55
1:A:105:ARG:NH2	1:A:109:LYS:HE3	2.21	0.54
1:B:260:LEU:HD21	1:B:294:TYR:HE2	1.72	0.54
1:B:273:LEU:HB2	1:B:283:GLN:HE22	1.71	0.54
1:A:44:PHE:CZ	1:A:474:LYS:HG3	2.42	0.54
1:A:105:ARG:HH12	1:A:109:LYS:CE	2.17	0.54
1:A:273:LEU:HB3	1:A:283:GLN:NE2	2.22	0.54
1:B:13:VAL:O	1:B:13:VAL:CG2	2.56	0.54
1:B:330:ILE:HG23	4:B:741:HOH:O	2.06	0.54
1:B:49:VAL:HG11	1:B:465:GLN:HA	1.89	0.54
1:B:480:ARG:HD2	4:B:708:HOH:O	2.06	0.54
1:A:100:GLN:OE1	1:A:263:LEU:HD21	2.06	0.54
1:B:60:THR:C	1:B:61:LEU:HD23	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ILE:HG22	1:B:222:ILE:HA	1.89	0.54
1:B:493:ARG:HG3	1:B:493:ARG:HH11	1.73	0.54
1:A:457:VAL:HB	1:A:458:PRO:HD3	1.90	0.53
1:A:312:ASN:HD22	1:A:312:ASN:N	2.06	0.53
1:B:101:ALA:HA	1:B:263:LEU:HD23	1.89	0.53
1:B:334:GLN:O	1:B:337:LEU:HD23	2.08	0.53
1:A:70:MET:SD	2:A:631:CPR:H8	2.49	0.53
1:A:345:THR:HG23	4:A:705:HOH:O	2.07	0.53
1:B:334:GLN:CB	1:B:337:LEU:HB3	2.28	0.53
1:B:455:LYS:C	1:B:458:PRO:HD2	2.33	0.53
1:A:49:VAL:HG11	1:A:465:GLN:HA	1.91	0.53
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.72	0.53
1:A:408:LEU:HD13	1:A:408:LEU:C	2.34	0.53
1:B:59:ILE:HG12	1:B:298:GLN:HG3	1.89	0.53
1:B:61:LEU:HD23	1:B:61:LEU:N	2.23	0.53
1:B:259:ARG:HB2	4:B:712:HOH:O	2.09	0.52
1:B:473:ALA:HA	1:B:478:GLN:NE2	2.20	0.52
1:A:277:GLN:HE21	1:A:277:GLN:HA	1.73	0.52
1:B:495:SER:C	1:B:497:ALA:H	2.17	0.52
1:A:60:THR:C	1:A:61:LEU:HD23	2.34	0.52
1:B:82:MET:HE1	1:B:390:LEU:HD13	1.92	0.52
1:B:21:GLN:C	1:B:23:LEU:H	2.18	0.52
1:B:305:VAL:H	1:B:309:GLN:HE21	1.52	0.52
1:B:333:THR:HG22	1:B:334:GLN:H	1.75	0.52
1:B:287:ILE:HD13	1:B:299:VAL:HG11	1.92	0.51
1:B:41:TYR:CE2	1:B:43:ASP:HB3	2.45	0.51
1:A:386:MET:HE3	1:A:389:LEU:HD23	1.90	0.51
1:B:370:VAL:HA	1:B:373:ILE:HD12	1.92	0.51
1:A:93:HIS:HB3	1:A:100:GLN:NE2	2.25	0.51
1:A:273:LEU:CB	1:A:283:GLN:HE22	2.24	0.51
1:A:373:ILE:HG23	1:A:384:VAL:HG21	1.93	0.51
1:B:21:GLN:HE21	1:B:22:GLN:N	2.08	0.51
1:B:269:ASP:HB3	4:B:706:HOH:O	2.10	0.51
1:B:323:VAL:HG23	1:B:361:VAL:HG13	1.92	0.51
1:B:341:ARG:HG2	1:B:342:PRO:HD2	1.91	0.51
1:B:103:GLU:OE1	1:B:106:LYS:HD3	2.10	0.51
1:B:18:LEU:HB3	1:B:22:GLN:HG3	1.92	0.51
1:A:337:LEU:O	1:A:338:ALA:C	2.54	0.50
1:A:375:LYS:O	1:A:379:LEU:HG	2.11	0.50
1:B:19:THR:H	1:B:22:GLN:CD	2.18	0.50
1:B:337:LEU:O	1:B:338:ALA:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:THR:OG1	1:B:497:ALA:HB2	2.12	0.50
1:B:493:ARG:NH1	1:B:493:ARG:HG3	2.27	0.50
1:A:473:ALA:CB	1:A:479:VAL:HG22	2.42	0.50
1:B:103:GLU:O	1:B:107:VAL:HG23	2.12	0.50
1:B:335:GLU:HG3	4:B:717:HOH:O	2.10	0.50
1:A:293:LYS:HE2	1:A:294:TYR:OH	2.11	0.50
1:B:51:LEU:HD12	1:B:461:ILE:HG23	1.94	0.50
1:B:305:VAL:HG11	1:B:325:MET:HB3	1.93	0.50
1:A:330:ILE:HG22	1:A:331:CYS:N	2.27	0.50
1:A:454:HIS:O	1:A:455:LYS:HE3	2.11	0.50
1:A:10:THR:HG22	1:A:12:TYR:H	1.77	0.50
1:B:494:THR:N	1:B:497:ALA:HB3	2.27	0.50
1:A:53:SER:OG	1:A:64:PRO:HB3	2.12	0.49
1:A:494:THR:OG1	1:A:497:ALA:CB	2.60	0.49
1:A:65:LEU:HD13	1:A:460:LEU:HD12	1.94	0.49
1:B:93:HIS:HB3	1:B:100:GLN:HE22	1.77	0.49
1:B:332:ILE:HG12	1:B:333:THR:N	2.17	0.49
1:A:21:GLN:C	1:A:23:LEU:H	2.20	0.49
1:A:273:LEU:HD11	1:A:287:ILE:HD13	1.93	0.49
1:A:305:VAL:HG11	1:A:325:MET:HB3	1.93	0.49
1:A:395:GLU:OE1	1:A:453:ILE:HG12	2.11	0.49
1:B:36:LEU:HG	1:B:493:ARG:HH11	1.78	0.49
1:B:93:HIS:ND1	1:B:250:ILE:HA	2.26	0.49
1:B:212:VAL:HA	1:B:219:VAL:N	2.27	0.49
1:B:332:ILE:CG1	1:B:333:THR:H	2.16	0.49
1:B:454:HIS:O	1:B:458:PRO:HG2	2.12	0.49
1:A:212:VAL:HA	1:A:219:VAL:N	2.27	0.49
1:A:13:VAL:O	1:A:13:VAL:CG2	2.60	0.49
1:A:461:ILE:O	1:A:465:GLN:HG3	2.13	0.48
1:A:80:ILE:HG12	1:A:107:VAL:HG13	1.95	0.48
1:A:234:PRO:HG2	1:A:235:LEU:HG	1.95	0.48
1:A:314:ILE:HA	1:A:318:VAL:CG2	2.43	0.48
1:B:80:ILE:HG12	1:B:107:VAL:HG13	1.94	0.48
1:A:63:THR:HG21	1:A:461:ILE:HD11	1.95	0.48
1:B:300:ILE:HD13	1:B:362:ILE:HD11	1.96	0.48
1:B:330:ILE:HG12	1:B:335:GLU:HG2	1.95	0.48
1:A:241:LYS:NZ	4:A:729:HOH:O	2.46	0.48
1:A:454:HIS:O	1:A:458:PRO:HG2	2.14	0.48
1:B:21:GLN:O	1:B:23:LEU:N	2.46	0.48
1:A:277:GLN:NE2	1:A:279:ASN:H	2.12	0.48
1:B:47:ASP:OD1	1:B:48:GLN:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PHE:CE2	1:A:474:LYS:HG3	2.49	0.47
1:B:392:ALA:HB1	1:B:449:ASP:OD2	2.14	0.47
1:A:334:GLN:HE21	1:A:334:GLN:HA	1.79	0.47
1:B:21:GLN:C	1:B:23:LEU:N	2.71	0.47
1:B:144:ILE:O	1:B:152:SER:N	2.47	0.47
1:B:255:ASP:OD1	1:B:255:ASP:N	2.36	0.47
1:B:289:TYR:CE1	1:B:293:LYS:HD3	2.49	0.47
1:B:70:MET:HE2	1:B:73:VAL:HG23	1.96	0.47
1:B:483:MET:HB3	1:B:488:LEU:CD2	2.43	0.47
1:A:386:MET:HE1	1:A:460:LEU:CD1	2.44	0.47
1:A:105:ARG:HB3	1:A:105:ARG:CZ	2.45	0.47
1:A:144:ILE:O	1:A:152:SER:N	2.47	0.47
1:A:283:GLN:O	1:A:287:ILE:HG12	2.14	0.47
1:A:337:LEU:HD12	1:A:339:CYS:N	2.24	0.47
1:A:345:THR:O	1:A:349:LYS:HG2	2.14	0.47
1:A:241:LYS:HE2	4:A:729:HOH:O	2.15	0.47
1:A:368:GLN:H	1:A:372:HIS:CD2	2.32	0.47
1:A:21:GLN:O	1:A:23:LEU:N	2.48	0.47
1:A:249:ALA:HB1	1:A:274:ASP:HB2	1.97	0.47
1:B:353:TYR:O	1:B:356:ARG:HB2	2.15	0.47
1:A:277:GLN:CA	1:A:277:GLN:NE2	2.76	0.46
1:B:274:ASP:OD1	3:B:702:NAD:N7N	2.48	0.46
1:B:480:ARG:O	1:B:484:TYR:HD2	1.98	0.46
1:A:293:LYS:HG2	1:A:294:TYR:CD2	2.50	0.46
1:A:455:LYS:C	1:A:458:PRO:HD2	2.41	0.46
1:B:83:ALA:O	1:B:236:ALA:HA	2.16	0.46
1:A:283:GLN:OE1	1:A:302:GLY:N	2.43	0.46
1:B:44:PHE:O	1:B:469:GLN:NE2	2.48	0.46
1:B:273:LEU:HD11	1:B:287:ILE:HD13	1.97	0.46
1:A:352:GLU:O	1:A:352:GLU:CD	2.59	0.46
1:A:395:GLU:CD	1:A:453:ILE:H	2.23	0.46
1:B:13:VAL:O	1:B:13:VAL:HG23	2.14	0.46
1:A:83:ALA:O	1:A:236:ALA:HA	2.15	0.46
1:A:278:GLY:HA3	1:A:302:GLY:HA3	1.98	0.46
1:A:291:LYS:HA	1:A:291:LYS:HZ3	1.79	0.46
1:A:312:ASN:N	1:A:312:ASN:ND2	2.64	0.46
1:B:45:THR:H	1:B:48:GLN:HE21	1.63	0.46
1:B:93:HIS:HB3	1:B:100:GLN:NE2	2.31	0.46
1:A:273:LEU:CB	1:A:283:GLN:NE2	2.80	0.45
1:A:471:ILE:HD11	1:A:479:VAL:HG13	1.96	0.45
1:B:457:VAL:HB	1:B:458:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:LYS:HG2	1:B:493:ARG:N	2.31	0.45
1:A:483:MET:CB	1:A:488:LEU:HD23	2.44	0.45
1:B:273:LEU:HB3	1:B:283:GLN:NE2	2.31	0.45
1:A:325:MET:HG2	1:A:340:GLY:HA2	1.97	0.45
1:B:104:VAL:HG21	1:B:263:LEU:HD22	1.99	0.45
1:A:85:THR:HB	1:A:457:VAL:HG11	1.98	0.45
1:A:146:ASP:O	1:A:148:GLY:N	2.50	0.45
1:A:333:THR:CG2	1:A:334:GLN:H	2.28	0.45
1:A:21:GLN:C	1:A:23:LEU:N	2.72	0.45
1:A:287:ILE:HD13	1:A:299:VAL:HG11	1.98	0.45
1:A:92:HIS:HD2	1:A:94:ASN:H	1.61	0.45
1:A:97:PRO:HG3	1:A:259:ARG:CZ	2.46	0.45
1:A:115:ILE:HG22	1:A:221:ILE:C	2.42	0.45
1:A:51:LEU:HD12	1:A:461:ILE:HG23	1.98	0.45
1:A:203:ARG:C	1:A:205:LYS:H	2.25	0.45
1:A:19:THR:HB	1:A:22:GLN:CG	2.44	0.45
1:A:93:HIS:HB3	1:A:100:GLN:HE22	1.81	0.45
1:A:12:TYR:C	1:A:13:VAL:HG13	2.42	0.45
1:A:13:VAL:O	1:A:13:VAL:HG22	2.17	0.45
1:A:103:GLU:O	1:A:107:VAL:HG23	2.17	0.45
1:A:241:LYS:CE	4:A:729:HOH:O	2.65	0.45
1:B:261:ASP:CG	1:B:294:TYR:HH	2.25	0.45
1:A:23:LEU:O	1:A:28:ASP:OD2	2.35	0.44
1:B:249:ALA:HB1	1:B:274:ASP:HB2	1.98	0.44
1:B:203:ARG:C	1:B:205:LYS:H	2.25	0.44
1:B:273:LEU:CB	1:B:283:GLN:NE2	2.81	0.44
1:B:456:PHE:O	1:B:459:TYR:HB3	2.16	0.44
1:A:18:LEU:HD22	1:A:18:LEU:N	2.33	0.44
1:A:49:VAL:HG11	1:A:468:CYS:HB2	2.00	0.44
1:B:82:MET:CE	1:B:390:LEU:HD13	2.48	0.44
1:B:146:ASP:O	1:B:148:GLY:N	2.49	0.44
1:B:242:LYS:HD2	1:B:242:LYS:H	1.83	0.44
1:A:84:LEU:HA	1:A:236:ALA:CB	2.48	0.44
1:B:68:SER:HA	1:B:69:PRO:HD3	1.85	0.44
1:B:242:LYS:C	1:B:243:GLN:HG3	2.43	0.44
1:A:475:SER:O	1:A:479:VAL:HG23	2.18	0.44
1:B:10:THR:HG22	1:B:12:TYR:N	2.32	0.44
1:B:278:GLY:HA3	1:B:302:GLY:HA3	1.98	0.44
1:A:289:TYR:HD2	1:A:290:ILE:N	2.15	0.44
1:B:53:SER:O	1:B:60:THR:HG23	2.18	0.44
1:B:395:GLU:H	1:B:395:GLU:CD	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ILE:HG23	1:A:457:VAL:HG23	1.99	0.44
1:B:51:LEU:HD22	1:B:476:LEU:HD11	1.99	0.44
1:A:483:MET:HE3	1:A:484:TYR:CE1	2.53	0.43
1:A:455:LYS:HE3	1:A:455:LYS:HA	2.00	0.43
1:B:20:ALA:O	1:B:24:PHE:HD2	2.01	0.43
1:B:23:LEU:O	1:B:28:ASP:OD2	2.36	0.43
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.83	0.43
1:B:341:ARG:HA	1:B:342:PRO:HD3	1.87	0.43
1:B:483:MET:HE3	1:B:484:TYR:CD2	2.52	0.43
1:B:63:THR:HG23	1:B:86:GLY:HA3	2.00	0.43
1:B:354:ALA:HB1	1:B:359:VAL:O	2.18	0.43
1:A:408:LEU:HD13	1:A:409:LYS:N	2.32	0.43
1:B:13:VAL:O	1:B:14:PRO:O	2.36	0.43
1:B:301:GLY:O	1:B:302:GLY:O	2.36	0.43
1:A:76:ALA:O	1:A:80:ILE:HG13	2.18	0.43
1:A:386:MET:CE	1:A:389:LEU:HD23	2.49	0.43
1:A:289:TYR:CD2	1:A:290:ILE:N	2.86	0.43
1:A:341:ARG:CG	1:A:342:PRO:HD2	2.49	0.43
1:B:53:SER:OG	1:B:64:PRO:HB3	2.19	0.43
1:A:45:THR:N	1:A:48:GLN:HE21	2.05	0.42
1:A:260:LEU:O	1:A:263:LEU:HB2	2.20	0.42
1:B:333:THR:CG2	1:B:334:GLN:H	2.30	0.42
1:A:277:GLN:HE22	1:A:279:ASN:H	1.67	0.42
1:A:301:GLY:O	1:A:302:GLY:O	2.38	0.42
1:B:292:ASP:O	1:B:295:PRO:HD3	2.18	0.42
1:A:101:ALA:HA	1:A:263:LEU:HD23	2.02	0.42
1:B:260:LEU:O	1:B:263:LEU:HB2	2.20	0.42
1:A:323:VAL:CG2	1:A:361:VAL:HG13	2.47	0.42
1:B:452:SER:O	1:B:455:LYS:HG2	2.20	0.42
1:A:272:VAL:HG13	1:A:272:VAL:O	2.20	0.42
1:B:105:ARG:NH1	1:B:109:LYS:HG2	2.29	0.42
1:A:108:LYS:NZ	1:A:239:ASP:OD2	2.46	0.42
1:A:353:TYR:O	1:A:356:ARG:HB2	2.20	0.42
1:B:233:TYR:HE2	1:B:454:HIS:CE1	2.37	0.42
1:A:23:LEU:O	1:A:23:LEU:HG	2.14	0.42
2:A:631:CPR:H8	2:A:631:CPR:H3'	2.02	0.42
1:B:390:LEU:O	1:B:393:THR:HG23	2.19	0.42
1:A:97:PRO:HB3	1:A:259:ARG:HA	2.02	0.42
1:A:330:ILE:HG22	1:A:331:CYS:H	1.85	0.42
1:A:334:GLN:O	1:A:337:LEU:HD23	2.20	0.42
1:A:367:ILE:HD13	1:A:372:HIS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ASP:OD2	2:B:631:CPR:O2'	2.35	0.42
1:A:378:ALA:O	1:A:483:MET:HG2	2.20	0.41
1:A:456:PHE:O	1:A:459:TYR:HB3	2.19	0.41
1:B:238:LYS:HA	1:B:243:GLN:O	2.20	0.41
1:B:311:LYS:HG2	1:B:315:ASP:OD2	2.20	0.41
1:A:449:ASP:CG	1:A:450:LYS:N	2.77	0.41
1:B:63:THR:HG21	1:B:461:ILE:HD11	2.02	0.41
1:A:388:SER:O	1:A:390:LEU:N	2.54	0.41
1:B:19:THR:O	1:B:22:GLN:HG2	2.20	0.41
1:A:238:LYS:HB2	1:A:238:LYS:HE2	1.73	0.41
1:A:354:ALA:HB1	1:A:359:VAL:O	2.20	0.41
1:A:44:PHE:O	1:A:469:GLN:NE2	2.53	0.41
1:A:281:ILE:HG23	1:A:282:PHE:N	2.35	0.41
1:A:305:VAL:HG22	1:A:309:GLN:NE2	2.36	0.41
1:A:487:GLU:HA	1:B:12:TYR:CE1	2.55	0.41
1:B:18:LEU:HB3	1:B:22:GLN:HE21	1.84	0.41
1:B:73:VAL:HG21	1:B:387:GLY:CA	2.51	0.41
1:B:330:ILE:HG22	1:B:331:CYS:N	2.36	0.41
1:A:305:VAL:HG22	1:A:309:GLN:HE22	1.85	0.41
1:B:331:CYS:HB2	2:B:631:CPR:HN1	1.76	0.41
1:B:377:LEU:HA	1:B:381:ALA:HB3	2.02	0.41
1:A:471:ILE:CD1	1:A:479:VAL:HG13	2.51	0.41
1:B:18:LEU:HA	1:B:22:GLN:NE2	2.35	0.41
1:A:23:LEU:HD23	1:A:24:PHE:CE2	2.56	0.41
1:A:45:THR:N	1:A:48:GLN:NE2	2.57	0.41
1:A:145:THR:HA	1:A:151:GLY:HA3	2.02	0.41
1:A:332:ILE:CG1	1:A:333:THR:N	2.76	0.41
1:B:115:ILE:HG22	1:B:221:ILE:C	2.46	0.41
1:B:388:SER:O	1:B:390:LEU:N	2.54	0.41
1:A:273:LEU:HB2	1:A:283:GLN:HE22	1.86	0.41
1:B:145:THR:HA	1:B:151:GLY:HA3	2.02	0.41
1:B:238:LYS:HB2	1:B:243:GLN:N	2.36	0.41
1:B:108:LYS:HD2	1:B:244:LEU:O	2.21	0.40
1:B:260:LEU:HD21	1:B:294:TYR:CE2	2.53	0.40
1:B:272:VAL:HG13	1:B:272:VAL:O	2.21	0.40
1:A:291:LYS:HA	1:A:291:LYS:CE	2.51	0.40
1:B:72:THR:HG22	1:B:411:TYR:CE1	2.56	0.40
1:B:51:LEU:HD21	1:B:464:ILE:HG22	2.04	0.40
1:B:388:SER:C	1:B:390:LEU:N	2.79	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	384/514 (75%)	304 (79%)	52 (14%)	28 (7%)	1	2
1	B	384/514 (75%)	301 (78%)	55 (14%)	28 (7%)	1	2
All	All	768/1028 (75%)	605 (79%)	107 (14%)	56 (7%)	1	2

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	147	THR
1	A	400	TYR
1	A	450	LYS
1	B	14	PRO
1	B	147	THR
1	B	400	TYR
1	B	450	LYS
1	A	17	GLY
1	A	145	THR
1	A	150	MET
1	A	302	GLY
1	A	337	LEU
1	A	451	GLY
1	B	17	GLY
1	B	145	THR
1	B	150	MET
1	B	302	GLY
1	B	337	LEU
1	B	451	GLY
1	A	13	VAL
1	A	22	GLN
1	A	27	GLY
1	A	236	ALA
1	B	13	VAL

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Mol	Chain	Res	Type
1	B	22	GLN
1	B	27	GLY
1	B	112	GLN
1	B	236	ALA
1	A	112	GLN
1	A	122	SER
1	A	207	GLY
1	A	289	TYR
1	B	207	GLY
1	B	289	TYR
1	B	344	ALA
1	A	110	TYR
1	A	149	ARG
1	A	338	ALA
1	A	344	ALA
1	A	389	LEU
1	A	399	GLU
1	A	405	GLY
1	B	122	SER
1	B	149	ARG
1	B	338	ALA
1	B	399	GLU
1	B	405	GLY
1	B	496	SER
1	A	340	GLY
1	B	110	TYR
1	B	340	GLY
1	B	389	LEU
1	B	305	VAL
1	A	305	VAL
1	A	318	VAL

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/420 (64%)	241 (89%)	30 (11%)	6	20
1	B	271/420 (64%)	241 (89%)	30 (11%)	6	20
All	All	542/840 (64%)	482 (89%)	60 (11%)	6	20

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	13	VAL
1	A	16	ASP
1	A	18	LEU
1	A	21	GLN
1	A	25	ASN
1	A	31	THR
1	A	38	LEU
1	A	61	LEU
1	A	75	GLU
1	A	111	GLU
1	A	255	ASP
1	A	259	ARG
1	A	261	ASP
1	A	277	GLN
1	A	291	LYS
1	A	298	GLN
1	A	329	SER
1	A	336	VAL
1	A	339	CYS
1	A	356	ARG
1	A	382	SER
1	A	386	MET
1	A	399	GLU
1	A	400	TYR
1	A	409	LYS
1	A	410	LYS
1	A	450	LYS
1	A	455	LYS
1	A	492	LYS
1	B	13	VAL
1	B	16	ASP

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Mol	Chain	Res	Type
1	B	18	LEU
1	B	21	GLN
1	B	38	LEU
1	B	61	LEU
1	B	63	THR
1	B	111	GLU
1	B	232	ASP
1	B	238	LYS
1	B	255	ASP
1	B	260	LEU
1	B	268	VAL
1	B	277	GLN
1	B	291	LYS
1	B	329	SER
1	B	334	GLN
1	B	336	VAL
1	B	339	CYS
1	B	356	ARG
1	B	386	MET
1	B	388	SER
1	B	394	THR
1	B	400	TYR
1	B	406	ILE
1	B	409	LYS
1	B	410	LYS
1	B	450	LYS
1	B	495	SER
1	B	498	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	48	GLN
1	A	92	HIS
1	A	94	ASN
1	A	112	GLN
1	A	265	GLN
1	A	277	GLN
1	A	309	GLN
1	A	312	ASN
1	A	334	GLN

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Mol	Chain	Res	Type
1	A	372	HIS
1	A	454	HIS
1	A	478	GLN
1	B	21	GLN
1	B	22	GLN
1	B	48	GLN
1	B	92	HIS
1	B	94	ASN
1	B	112	GLN
1	B	265	GLN
1	B	309	GLN
1	B	312	ASN
1	B	368	GLN
1	B	372	HIS
1	B	454	HIS
1	B	478	GLN
1	B	498	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	B	702	-	46,48,48	1.99	11 (23%)	64,73,73	1.59	9 (14%)
2	CPR	A	631	-	24,24,25	1.28	3 (12%)	33,36,38	2.00	7 (21%)
3	NAD	A	701	-	46,48,48	1.91	11 (23%)	64,73,73	1.65	11 (17%)
2	CPR	B	631	-	24,24,25	1.28	3 (12%)	33,36,38	2.00	8 (24%)

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	B	702	-	-	11/30/62/62	0/5/5/5
2	CPR	A	631	-	-	3/10/26/26	0/3/3/3
3	NAD	A	701	-	-	11/30/62/62	0/5/5/5
2	CPR	B	631	-	-	3/10/26/26	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NAD	C2N-N1N	5.71	1.41	1.35
3	A	701	NAD	C2N-N1N	5.14	1.40	1.35
3	B	702	NAD	O4D-C1D	4.94	1.47	1.40
3	A	701	NAD	O4D-C1D	4.91	1.47	1.40
3	B	702	NAD	C6N-N1N	4.73	1.46	1.35
3	A	701	NAD	C6N-N1N	4.71	1.46	1.35
3	B	702	NAD	PN-O3	4.17	1.64	1.59
3	A	701	NAD	PN-O3	3.95	1.63	1.59
3	B	702	NAD	PA-O3	3.77	1.63	1.59
3	A	701	NAD	PA-O3	3.29	1.63	1.59
2	B	631	CPR	C6-N1	3.18	1.34	1.31
3	B	702	NAD	C5A-N7A	-3.17	1.33	1.39
3	A	701	NAD	C5A-N7A	-3.16	1.33	1.39
2	A	631	CPR	C6-N1	2.89	1.34	1.31
3	A	701	NAD	O4B-C1B	2.83	1.48	1.42
3	B	702	NAD	O4B-C1B	2.75	1.48	1.42
2	A	631	CPR	C5-N7	-2.69	1.32	1.39
2	B	631	CPR	C5-N7	-2.58	1.32	1.39
3	A	701	NAD	C4A-N9A	-2.54	1.32	1.37
3	B	702	NAD	C4N-C3N	2.50	1.43	1.39
3	B	702	NAD	C4A-N9A	-2.49	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NAD	C5N-C4N	2.38	1.43	1.38
3	A	701	NAD	C4N-C3N	2.35	1.43	1.39
3	A	701	NAD	C6N-C5N	2.33	1.43	1.38
2	A	631	CPR	O4'-C1'	2.29	1.47	1.42
3	B	702	NAD	C6N-C5N	2.23	1.43	1.38
3	A	701	NAD	C5N-C4N	2.21	1.42	1.38
2	B	631	CPR	O4'-C1'	2.14	1.46	1.42

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAD	N3A-C2A-N1A	-5.96	119.57	128.58
3	B	702	NAD	N3A-C2A-N1A	-5.94	119.59	128.58
2	A	631	CPR	C2-N3-C4	5.49	120.58	111.14
2	B	631	CPR	C2-N3-C4	5.39	120.42	111.14
2	A	631	CPR	C5-C4-N3	-4.96	119.81	127.24
2	B	631	CPR	C5-C4-N3	-4.91	119.88	127.24
3	A	701	NAD	C5A-C4A-N3A	-4.67	120.29	126.72
3	B	702	NAD	C5A-C4A-N3A	-4.65	120.31	126.72
2	B	631	CPR	C6-N1-C2	4.43	121.41	115.77
2	A	631	CPR	C6-N1-C2	4.40	121.37	115.77
2	A	631	CPR	N1-C2-N3	-4.38	120.64	128.84
2	B	631	CPR	N1-C2-N3	-4.35	120.70	128.84
3	A	701	NAD	C2A-N3A-C4A	3.98	121.55	111.83
3	B	702	NAD	C2A-N3A-C4A	3.96	121.50	111.83
3	B	702	NAD	N9A-C8A-N7A	-3.21	109.38	113.94
3	A	701	NAD	N9A-C8A-N7A	-3.21	109.39	113.94
3	A	701	NAD	C3N-C7N-N7N	-3.06	113.96	117.74
3	A	701	NAD	N3A-C4A-N9A	3.05	132.35	127.17
3	B	702	NAD	N3A-C4A-N9A	3.03	132.32	127.17
2	A	631	CPR	C8-N7-C5	2.89	107.90	104.92
3	A	701	NAD	C6N-N1N-C2N	-2.89	119.42	121.88
2	B	631	CPR	C8-N7-C5	2.76	107.77	104.92
3	B	702	NAD	C6N-N1N-C2N	-2.71	119.58	121.88
3	A	701	NAD	C5A-N7A-C8A	2.65	107.61	103.45
3	B	702	NAD	C5A-N7A-C8A	2.61	107.55	103.45
2	B	631	CPR	N9-C4-N3	2.58	132.78	126.90
3	A	701	NAD	C4A-C5A-N7A	-2.57	107.65	110.58
3	B	702	NAD	C4A-C5A-N7A	-2.50	107.73	110.58
2	A	631	CPR	N9-C4-N3	2.49	132.57	126.90
3	A	701	NAD	O7N-C7N-C3N	2.38	122.50	119.60
2	A	631	CPR	N9-C8-N7	-2.29	109.15	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	631	CPR	N9-C8-N7	-2.26	109.20	113.40
3	A	701	NAD	C4A-N9A-C8A	2.15	108.00	105.74
3	B	702	NAD	C4A-N9A-C8A	2.14	107.98	105.74
2	B	631	CPR	O2P-P-O1P	2.00	118.64	110.83

There are no chirality outliers.

All (28) torsion outliers are listed below:

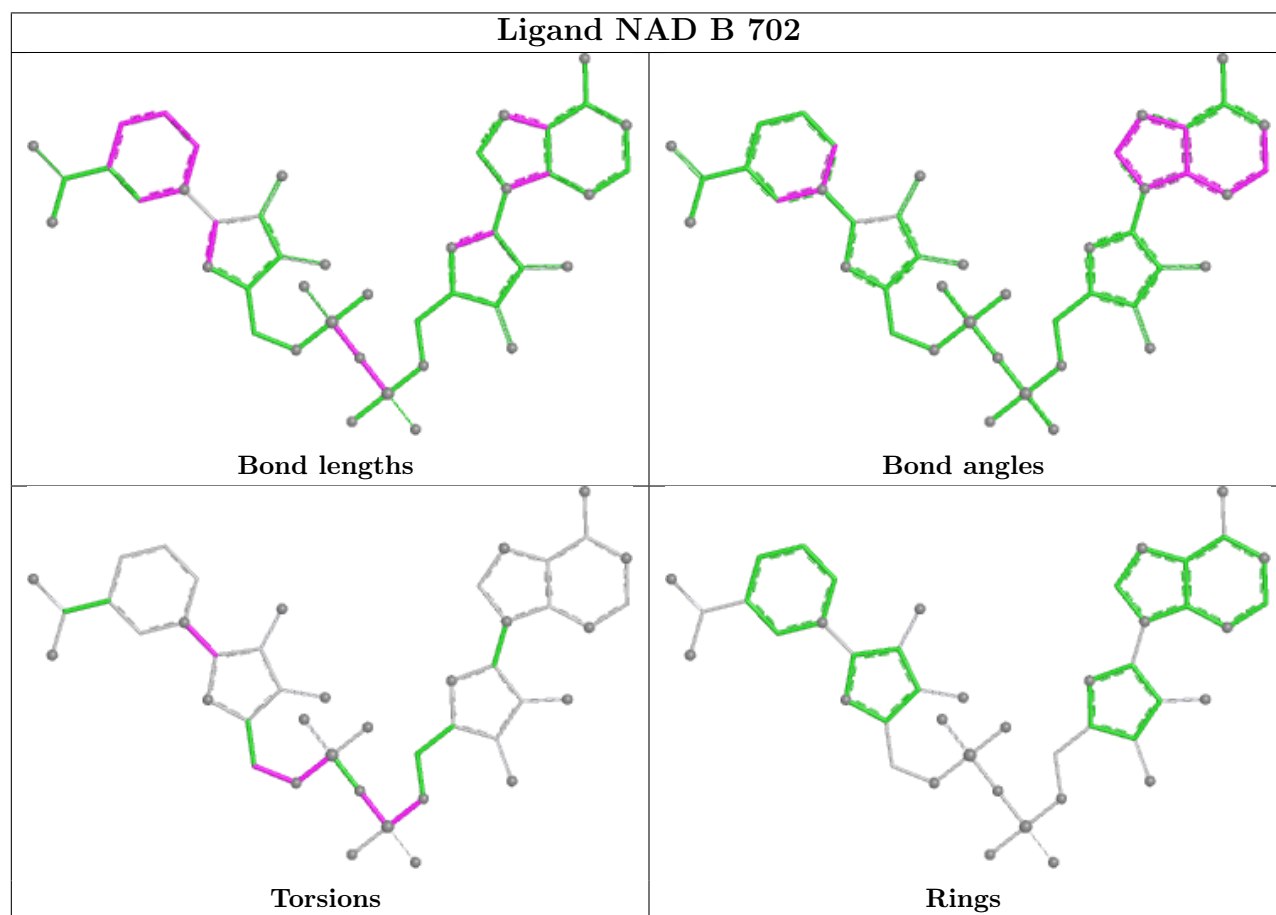
Mol	Chain	Res	Type	Atoms
2	A	631	CPR	C5'-O5'-P-O1P
2	A	631	CPR	C5'-O5'-P-O2P
2	A	631	CPR	C5'-O5'-P-O3P
2	B	631	CPR	C5'-O5'-P-O1P
2	B	631	CPR	C5'-O5'-P-O2P
2	B	631	CPR	C5'-O5'-P-O3P
3	A	701	NAD	C5D-O5D-PN-O1N
3	A	701	NAD	C4D-C5D-O5D-PN
3	A	701	NAD	C2D-C1D-N1N-C6N
3	B	702	NAD	C5D-O5D-PN-O1N
3	B	702	NAD	C4D-C5D-O5D-PN
3	B	702	NAD	C2D-C1D-N1N-C6N
3	A	701	NAD	C5B-O5B-PA-O1A
3	A	701	NAD	C5B-O5B-PA-O2A
3	A	701	NAD	C5B-O5B-PA-O3
3	A	701	NAD	C5D-O5D-PN-O3
3	A	701	NAD	C5D-O5D-PN-O2N
3	B	702	NAD	C5B-O5B-PA-O1A
3	B	702	NAD	C5B-O5B-PA-O2A
3	B	702	NAD	C5B-O5B-PA-O3
3	B	702	NAD	C5D-O5D-PN-O3
3	B	702	NAD	C5D-O5D-PN-O2N
3	A	701	NAD	C2D-C1D-N1N-C2N
3	B	702	NAD	C2D-C1D-N1N-C2N
3	A	701	NAD	PN-O3-PA-O1A
3	B	702	NAD	PN-O3-PA-O1A
3	A	701	NAD	PN-O3-PA-O2A
3	B	702	NAD	PN-O3-PA-O2A

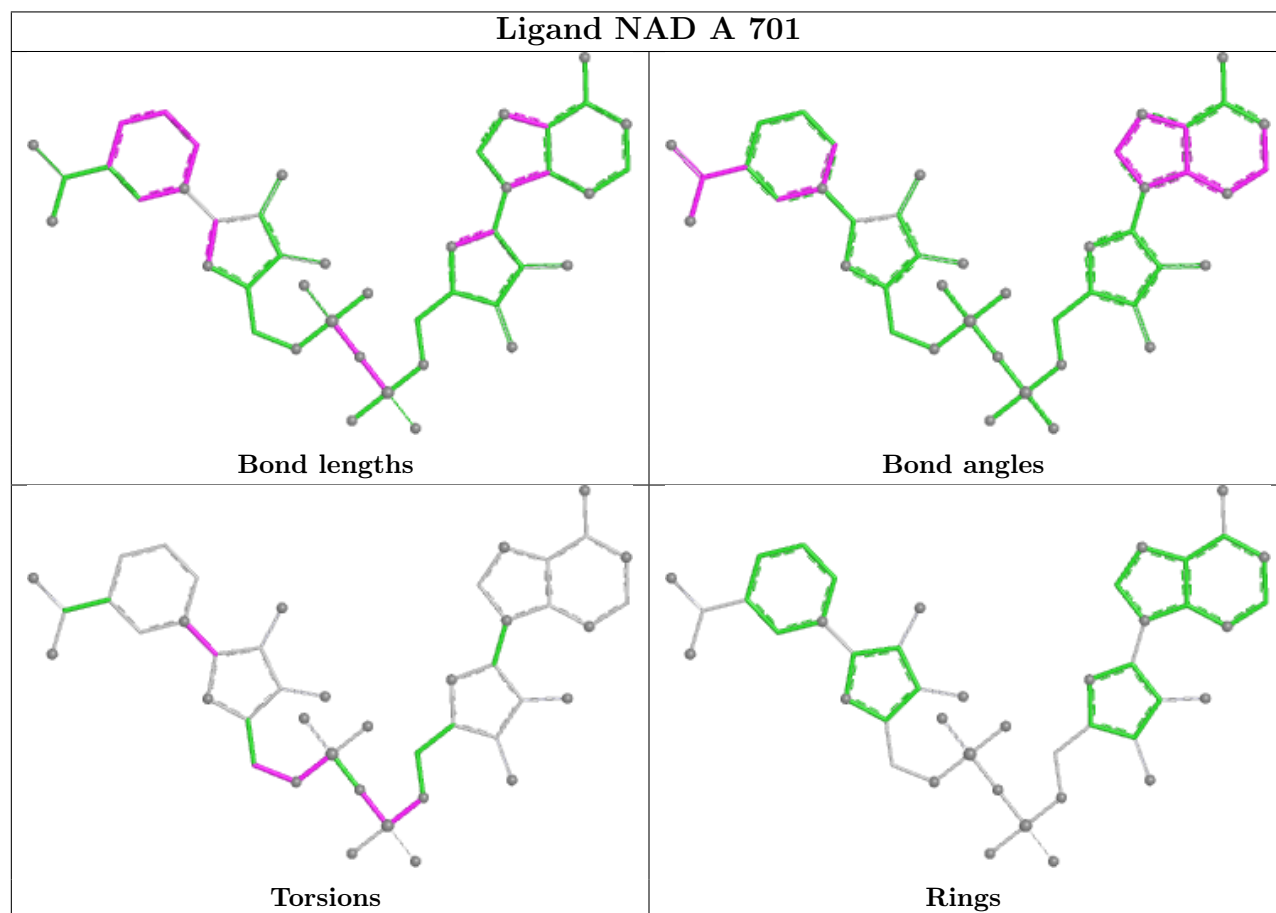
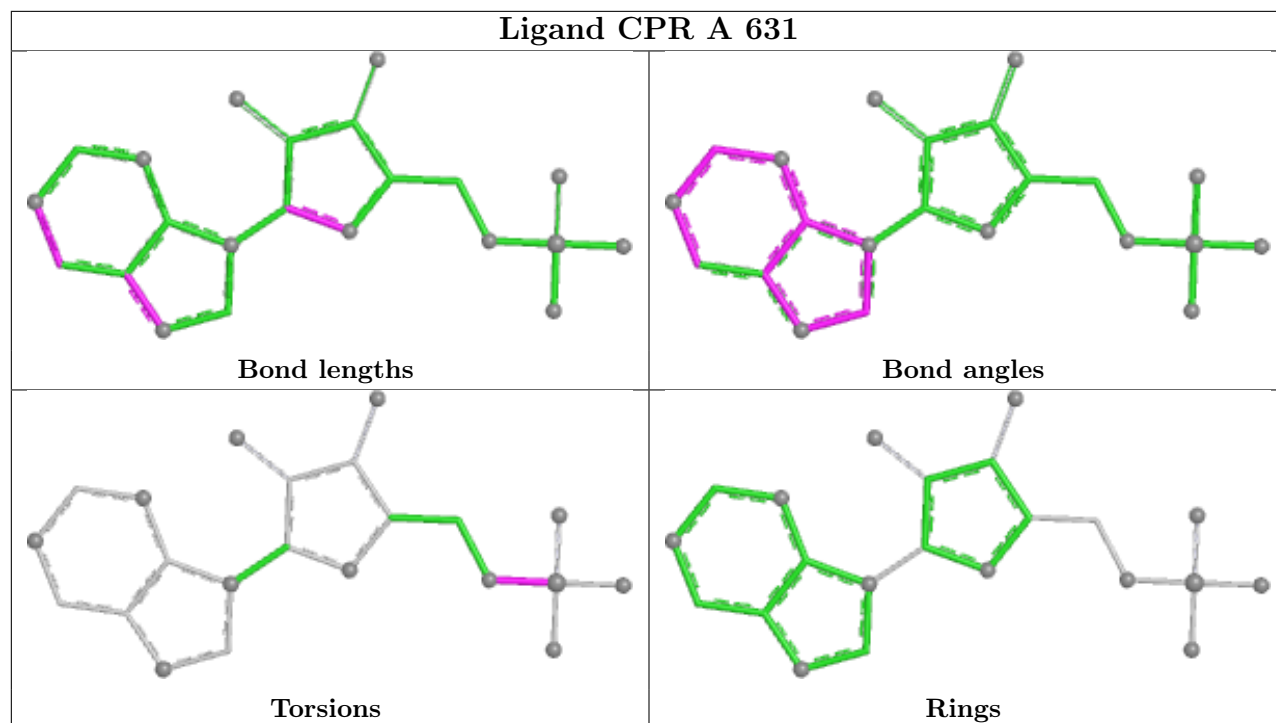
There are no ring outliers.

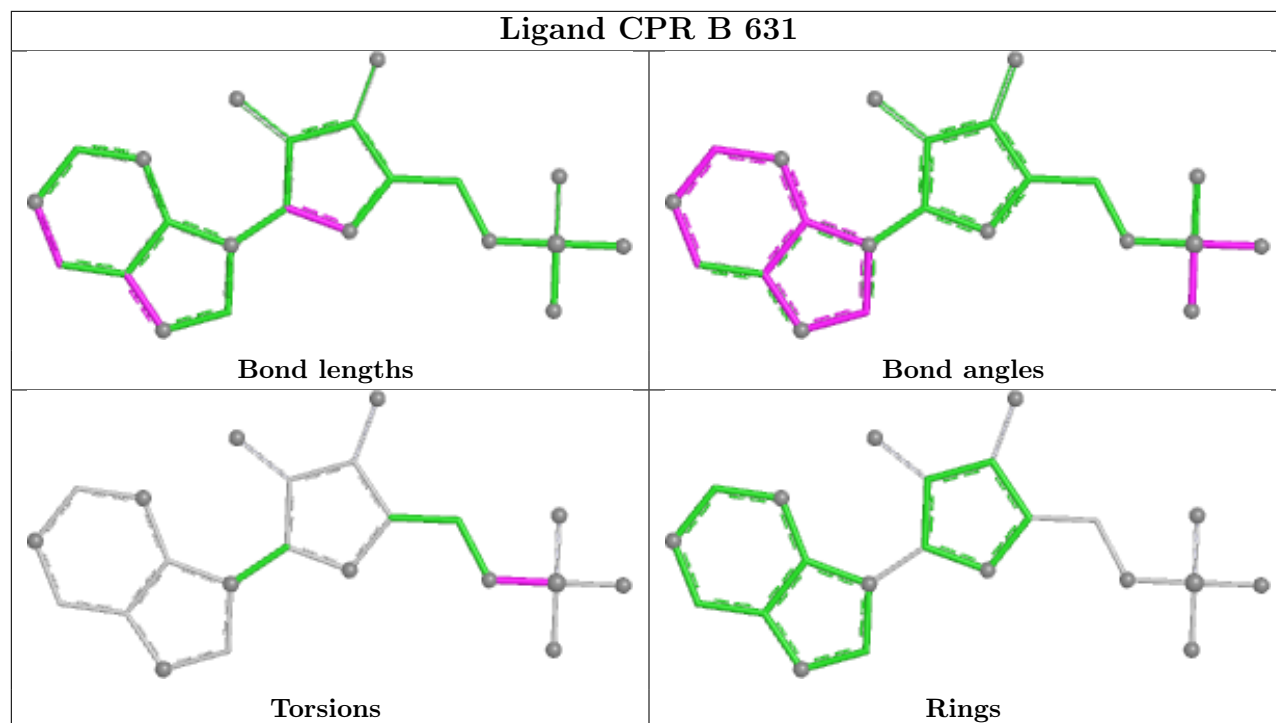
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	NAD	5	0
2	A	631	CPR	2	0
3	A	701	NAD	4	0
2	B	631	CPR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	396/514 (77%)	-1.02	1 (0%) 90 87	18, 52, 110, 143	0
1	B	396/514 (77%)	-1.05	2 (0%) 87 83	17, 52, 112, 148	0
All	All	792/1028 (77%)	-1.03	3 (0%) 88 85	17, 52, 111, 148	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	403	SER	5.4
1	B	267	GLY	2.8
1	A	152	SER	2.3

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(Å ²)	Q<0.9
3	NAD	A	701	44/44	0.98	0.08	126,126,126,126	0
3	NAD	B	702	44/44	0.98	0.09	138,138,138,138	0

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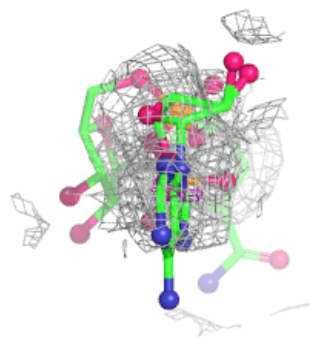
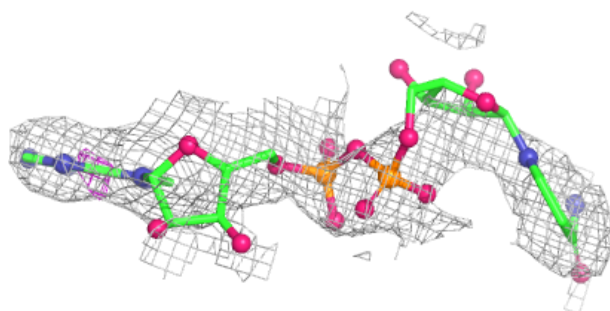
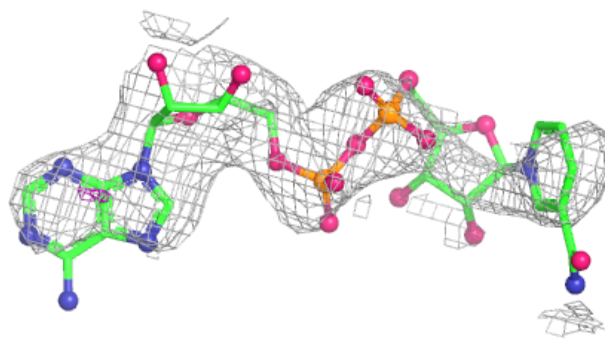
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CPR	A	631	22/23	0.99	0.04	74,75,75,76	0
2	CPR	B	631	22/23	0.99	0.04	69,70,70,70	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.

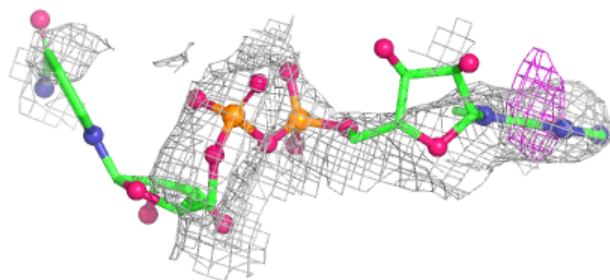
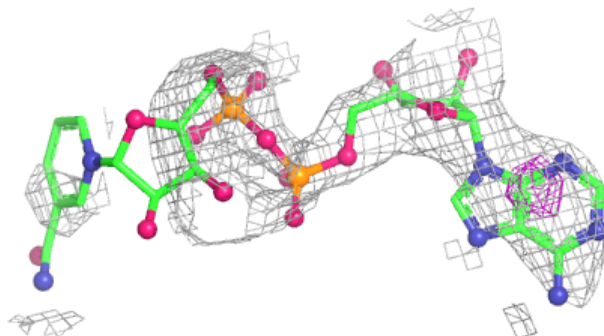
Electron density around NAD A 701:

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

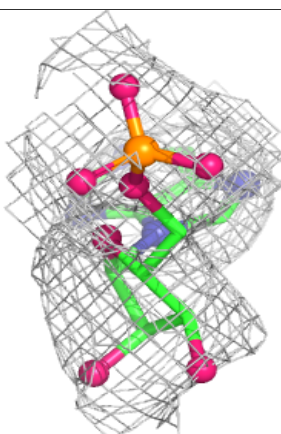
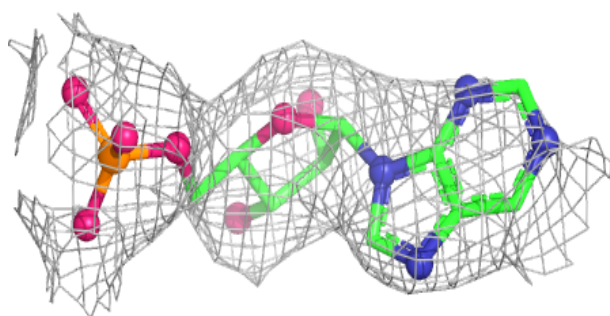
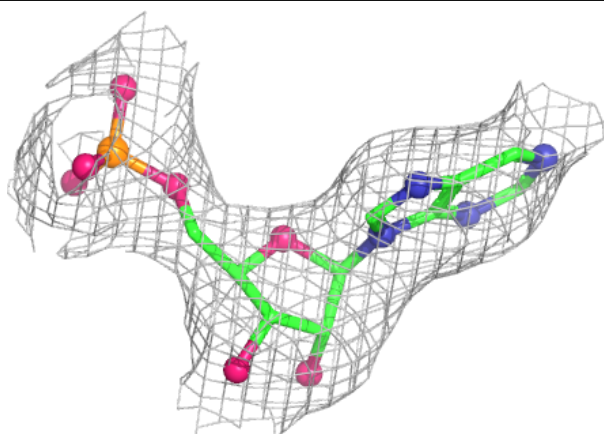


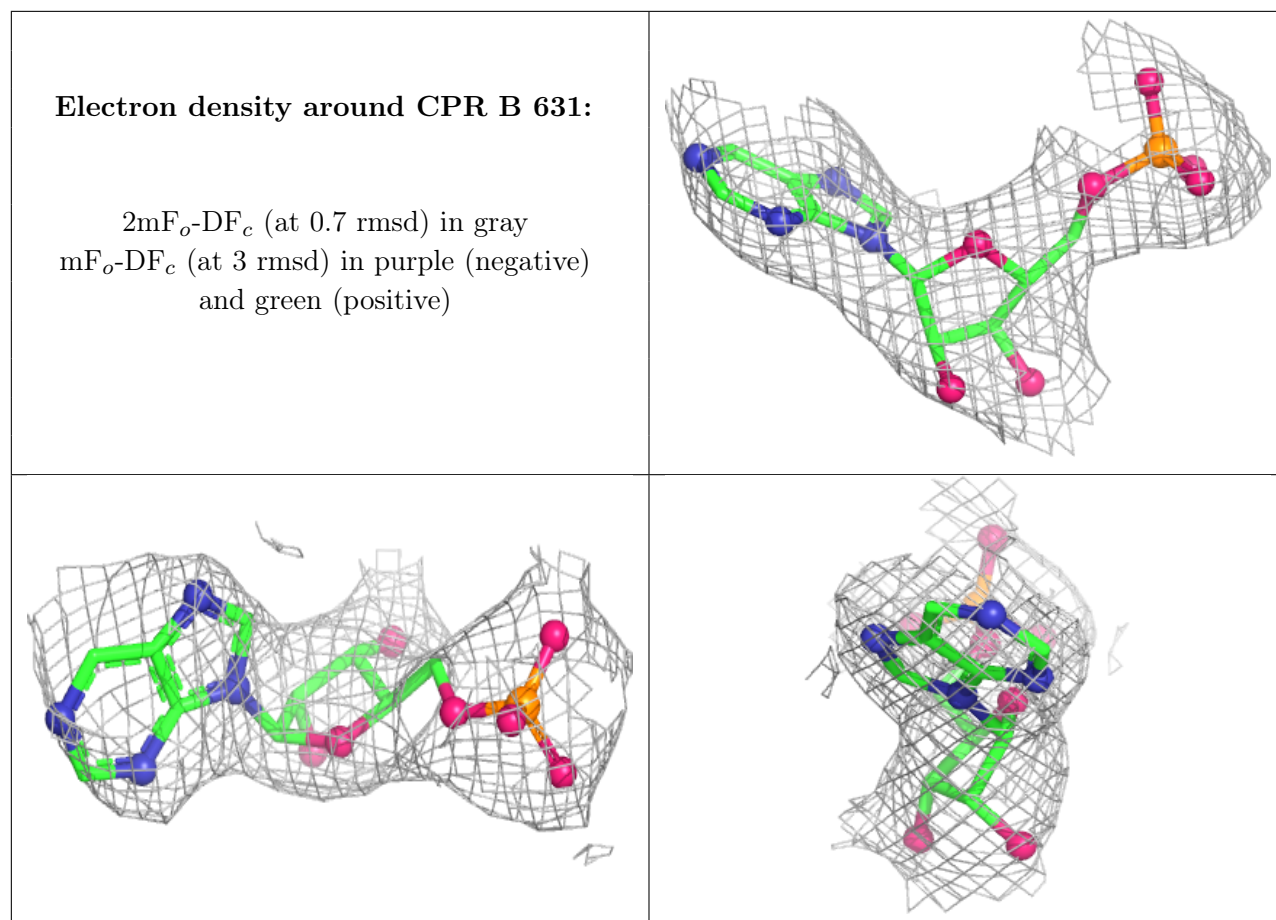
Electron density around NAD B 702:

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

**Electron density around CPR A 631:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.