Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 05:31 PM EDT

PDB ID	:	1NFB
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 (i) 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 (i)) were used in the production of this report:

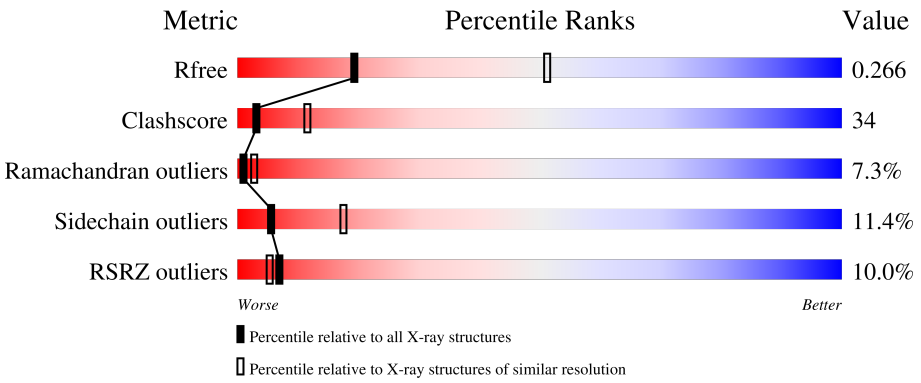
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	8% 37% 34% 6% 23%
1	B	514	8% 37% 34% 6% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAD	B	702	-	-	-	X

2 Entry composition (i)

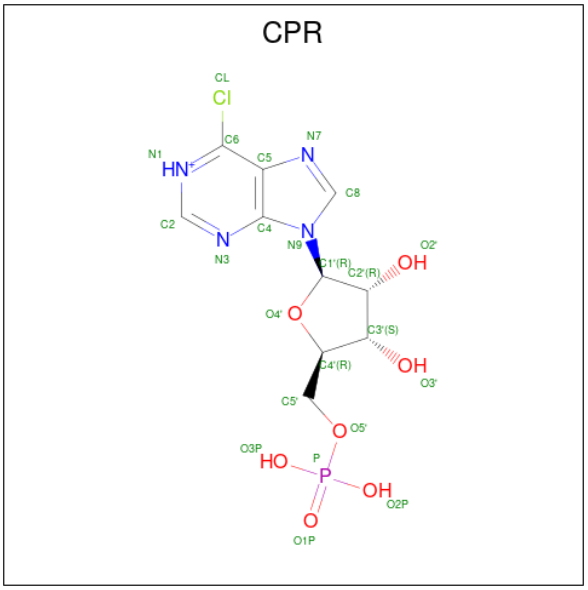
There are 4 unique types of molecules in this entry. The entry contains 5885 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	396	2833	1783	489	545	16	0	0	0
1	B	396	2833	1783	489	545	16	0	0	0

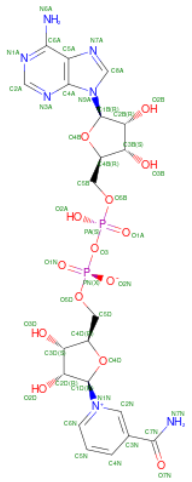
- Molecule 2 is 6-CHLOROPURINE RIBOSIDE, 5'-MONOPHOSPHATE (three-letter code: CPR) (formula: $C_{10}H_{13}ClN_4O_7P$).



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

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

NAD



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

- Molecule 4 is water.

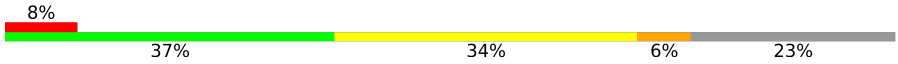
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	43	43	43	0	0
			Total	O		
4	B	44	44	44	0	0

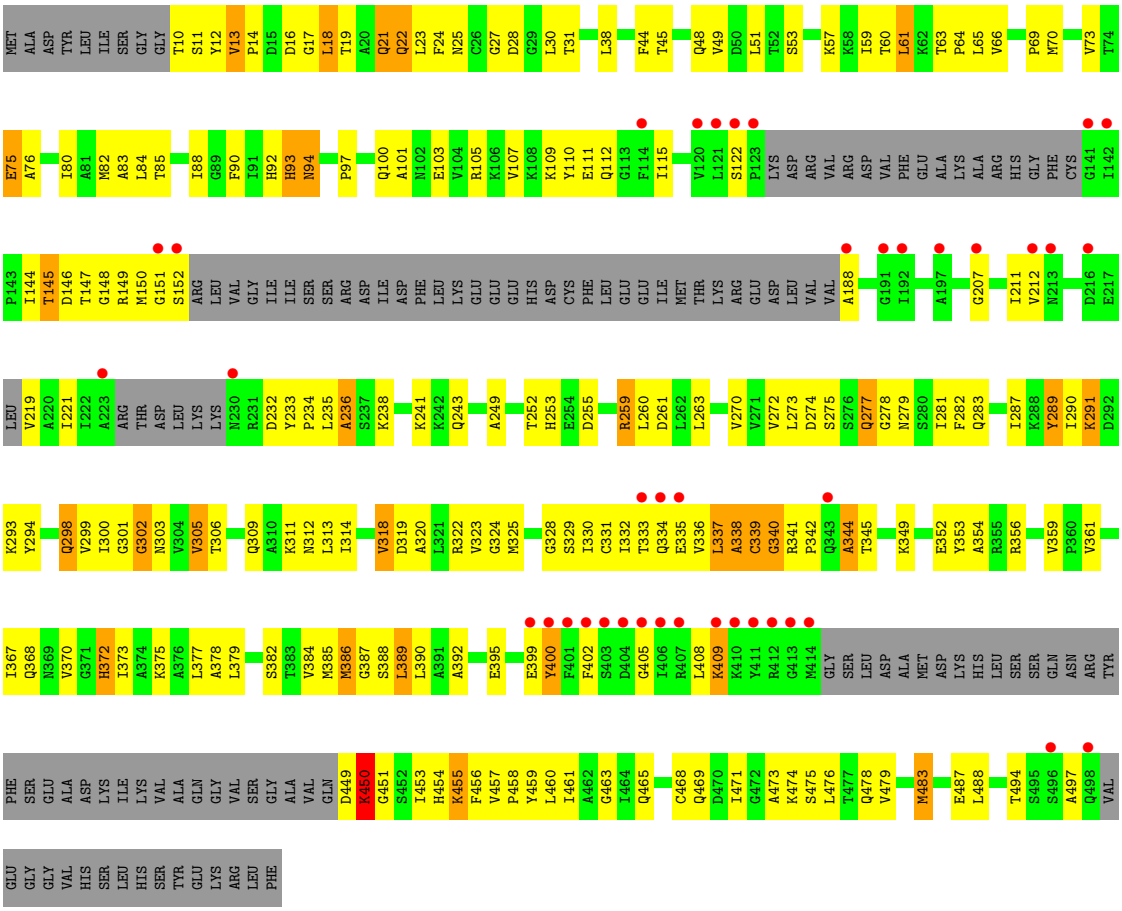
3 Residue-property plots (i)

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

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

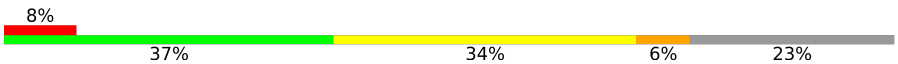
Chain A:

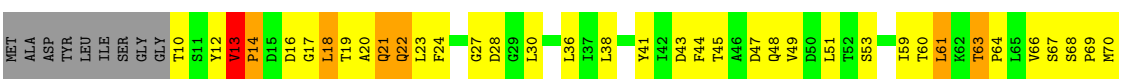


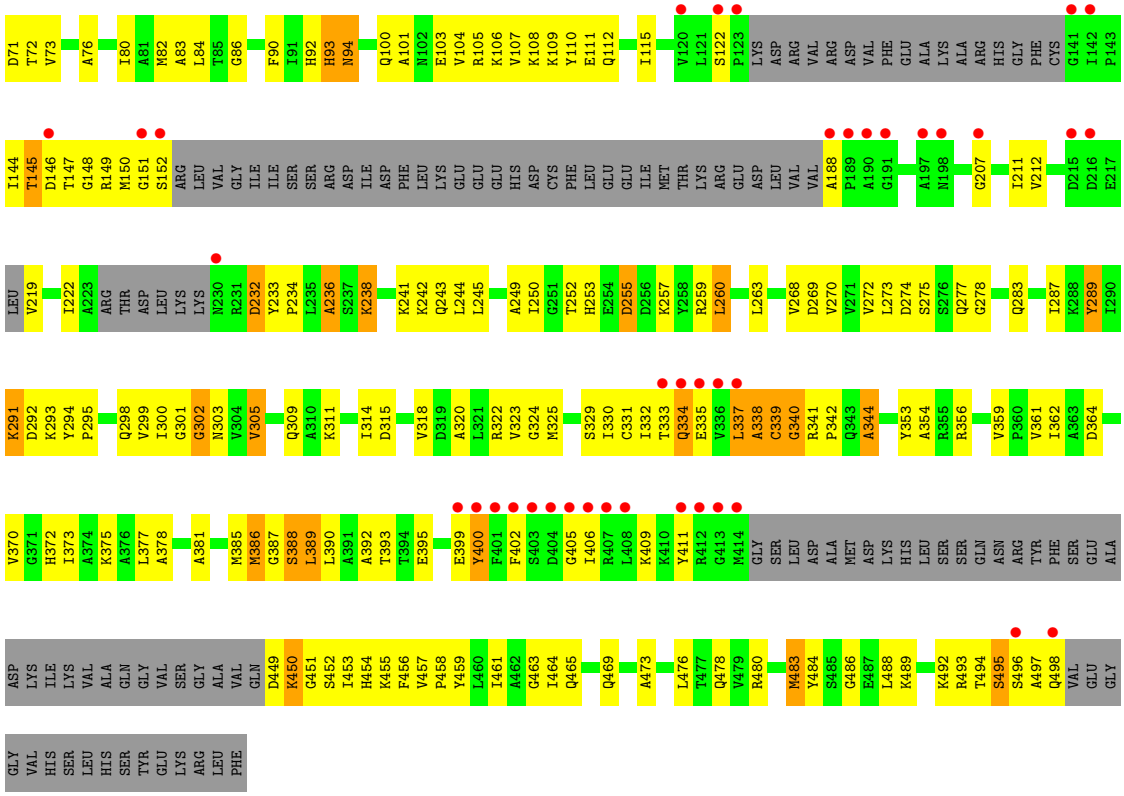


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain B:






D71 T72 V73 A76 I80 A81 M82 A83 L84 T85 G86 F90 I91 H92 H93 N94 Q100 A101 N102 E103 V104 R105 K106 V107 K108 K109 Y110 E111 Q112 I115 V120 L121 S122 P123 LYS ASP ARG VAL ARG ASP VAL PHE GLU ALA LYS ALA ARG HIS GLY PHE CYS G141 I142 P143
I144 T145 D146 T147 G148 R149 M150 G151 S152 ARG LEU VAL GLY ILE ILE SER SER ARG ASP ILE ASP PHE LEU LYS GLU GLU GLU HIS ASP CYS PHE LEU GLU GLU ILE MET THR LYS ARG GLU ASP LEU VAL VAL A188 P189 A190 G191 A197 N198 G207 I211 V212 D215 D216 E217
LEU V219 I222 A223 ARG THR ASP LEU LYS LYS N230 R231 D232 Y233 P234 L235 A236 S237 K238 K241 K242 Q243 L244 L245 A249 I250 G251 T252 H253 E254 D255 D256 K257 Y258 R259 L260 L263 V268 D269 V270 V271 V272 L273 D274 S275 S276 Q277 G278 Q283 I287 K288 Y289 I290
K291 D292 K293 Y294 P295 Q298 V299 I300 G301 G302 N303 V304 V305 Q309 A310 K311 I314 D315 V318 D319 A320 L321 R322 V323 G324 M325 S329 I330 C331 I332 T333 Q334 E335 V336 L337 A338 G339 G340 R341 P342 Q343 A344 Y353 A354 R355 R356 V359 P360 V361 I362 A363 D364
V370 G371 H372 I373 A374 K375 A376 L377 A378 A381 M385 M386 G387 S388 L389 L390 A391 A392 T393 T394 E395 E399 Y400 F401 F402 S403 D404 G405 I406 R407 L408 K409 K410 Y411 R412 G413 M414 GLY SER LEU ASP ALA MET ASP LYS HIS LEU SER SER GLN ASN ARG TYR PHE SER GLU ALA
ASP LYS ILE LYS VAL ALA GLN GLY VAL SER GLY ALA VAL GLN D449 K450 G451 S452 I453 H454 K455 F456 V457 P458 Y459 L460 I461 A462 G463 I464 Q465 Q469 A473 L476 T477 Q478 V479 R480 M483 Y484 S485 G486 E487 L488 K489 K492 R493 T494 S495 S496 A497 Q498 VAL GLU GLY
GLY VAL HIS SER LEU HIS SER TYR GLU LYS ARG LEU PHE

4 Data and refinement statistics (i)

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 51.33 – 2.90	Depositor EDS
% Data completeness (in resolution range)	66.5 (47.82-2.90) 74.6 (51.33-2.90)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	0.74 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.274 0.245 , 0.266	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 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.447 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.49	0/2870	0.74	1/3881 (0.0%)
1	B	0.50	0/2870	0.75	0/3881
All	All	0.49	0/5740	0.75	1/7762 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	450	LYS	CB-CG-CD	5.17	125.05	111.60

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	2833	0	2702	189	0
1	B	2833	0	2702	186	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	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5885	0	5478	379	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 34.

All (379) 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: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: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: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:82:MET:HE3	1:B:390:LEU:HD13	1.69	0.74
1:B:303:ASN:OD1	1:B:322:ARG:HD3	1.87	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:82:MET:HE3	1:A:390:LEU:HD13	1.78	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:HG21	1:B:283:GLN:HG2	1.86	0.57
1:A:277:GLN:HE21	1:A:277:GLN:C	2.09	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:67:SER:HB3	1:B:82:MET:HE3	1.87	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:B:386:MET:HE3	1:B:389:LEU:HD23	1.88	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:A:386:MET:HE2	1:A:389:LEU:HD23	1.90	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:B:483:MET:HE3	1:B:484:TYR:CZ	2.42	0.54
1:A:100:GLN:OE1	1:A:263:LEU:HD21	2.06	0.54
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:HG12	1:B:298:GLN:HG3	1.89	0.53
1:B:61:LEU:N	1:B:61:LEU:HD23	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: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: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:82:MET:HE3	1:B:390:LEU:CD1	2.39	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:375:LYS:O	1:A:379:LEU:HG	2.11	0.50
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:B:386:MET:HE1	1:B:389:LEU:HD23	1.94	0.49
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:60:THR:C	1:B:61:LEU:HD23	2.33	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:455:LYS:C	1:B:458:PRO:HD2	2.33	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:A:408:LEU:HD13	1:A:408:LEU:C	2.34	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:495:SER:C	1:B:497:ALA:H	2.17	0.48
1:B:47:ASP:OD1	1:B:48:GLN:HG3	2.14	0.48
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:60:THR:C	1:A:61:LEU:HD23	2.34	0.47
1:A:334:GLN:HE21	1:A:334:GLN:HA	1.79	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:483:MET:HB3	1:B:488:LEU:CD2	2.43	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:B:21:GLN:C	1:B:23:LEU:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:83:ALA:O	1:B:236:ALA:HA	2.16	0.46
1:B:19:THR:H	1:B:22:GLN:CD	2.18	0.46
1:A:283:GLN:OE1	1:A:302:GLY:N	2.43	0.46
1:A:337:LEU:O	1:A:338:ALA:C	2.54	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:B:337:LEU:O	1:B:338:ALA:C	2.54	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:23:LEU:O	1:A:23:LEU:HG	2.14	0.45
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
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:287:ILE:HD13	1:A:299:VAL:HG11	1.98	0.45
1:B:483:MET:HE3	1:B:484:TYR:CE1	2.52	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:51:LEU:HD12	1:A:461:ILE:HG23	1.98	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:B:67:SER:HB3	1:B:82:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLN:C	1:A:23:LEU:H	2.20	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: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: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: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: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: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: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: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:70:MET:HB3	1:B:70:MET:HE2	1.85	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:B:21:GLN:C	1:B:23:LEU:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:395:GLU:CD	1:A:453:ILE:H	2.23	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
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:B:63:THR:HG21	1:B:461:ILE:HD11	2.02	0.41
1:A:21:GLN:C	1:A:23:LEU:N	2.72	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:455:LYS:C	1:A:458:PRO:HD2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:352:GLU:O	1:A:352:GLU:CD	2.59	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:375:LYS:NZ	4:B:709:HOH:O	2.53	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:A:115:ILE:HG22	1:A:221:ILE:C	2.42	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

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	384/514 (75%)	304 (79%)	52 (14%)	28 (7%)	1 3
1	B	384/514 (75%)	301 (78%)	55 (14%)	28 (7%)	1 3
All	All	768/1028 (75%)	605 (79%)	107 (14%)	56 (7%)	1 3

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
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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	271/420 (64%)	240 (89%)	31 (11%)	5 17
1	B	271/420 (64%)	240 (89%)	31 (11%)	5 17
All	All	542/840 (64%)	480 (89%)	62 (11%)	5 17

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
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	93	HIS

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Mol	Chain	Res	Type
1	A	94	ASN
1	A	111	GLU
1	A	232	ASP
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	372	HIS
1	A	382	SER
1	A	386	MET
1	A	400	TYR
1	A	402	PHE
1	A	409	LYS
1	A	450	LYS
1	A	455	LYS
1	A	483	MET
1	B	13	VAL
1	B	16	ASP
1	B	18	LEU
1	B	21	GLN
1	B	38	LEU
1	B	61	LEU
1	B	63	THR
1	B	93	HIS
1	B	94	ASN
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	339	CYS
1	B	372	HIS

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Mol	Chain	Res	Type
1	B	386	MET
1	B	388	SER
1	B	400	TYR
1	B	402	PHE
1	B	406	ILE
1	B	409	LYS
1	B	450	LYS
1	B	483	MET
1	B	495	SER
1	B	498	GLN

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	33	ASN
1	A	48	GLN
1	A	92	HIS
1	A	94	ASN
1	A	112	GLN
1	A	243	GLN
1	A	265	GLN
1	A	277	GLN
1	A	309	GLN
1	A	312	ASN
1	A	334	GLN
1	A	372	HIS
1	A	454	HIS
1	A	478	GLN
1	B	21	GLN
1	B	22	GLN
1	B	33	ASN
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	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 monosaccharides 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	-	42,48,48	1.83	6 (14%)	50,73,73	1.42	6 (12%)
3	NAD	A	701	-	42,48,48	1.79	6 (14%)	50,73,73	1.50	7 (14%)
2	CPR	A	631	1	20,24,25	1.38	1 (5%)	21,36,38	1.73	3 (14%)
2	CPR	B	631	1	20,24,25	1.34	1 (5%)	21,36,38	1.76	3 (14%)

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	-	-	11/26/62/62	0/5/5/5
3	NAD	A	701	-	-	11/26/62/62	0/5/5/5
2	CPR	A	631	1	-	3/6/26/26	0/3/3/3
2	CPR	B	631	1	-	3/6/26/26	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	NAD	O4B-C1B	5.35	1.48	1.41
3	B	702	NAD	O4B-C1B	5.22	1.48	1.41
3	B	702	NAD	C2N-N1N	5.17	1.41	1.35
3	A	701	NAD	C2N-N1N	4.66	1.40	1.35
3	B	702	NAD	O4D-C1D	4.52	1.47	1.41
3	A	701	NAD	O4D-C1D	4.48	1.47	1.41
2	A	631	CPR	O4'-C1'	4.45	1.47	1.41
3	B	702	NAD	C6N-N1N	4.39	1.46	1.35
3	A	701	NAD	C6N-N1N	4.37	1.46	1.35
2	B	631	CPR	O4'-C1'	4.20	1.46	1.41
3	B	702	NAD	C4N-C3N	2.28	1.43	1.39
3	A	701	NAD	C6N-C5N	2.19	1.43	1.38
3	A	701	NAD	C4N-C3N	2.14	1.43	1.39
3	B	702	NAD	C6N-C5N	2.09	1.43	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	NAD	N3A-C2A-N1A	-5.83	119.57	128.68
3	B	702	NAD	N3A-C2A-N1A	-5.81	119.59	128.68
2	A	631	CPR	N1-C2-N3	-5.47	120.64	127.65
2	B	631	CPR	N1-C2-N3	-5.43	120.70	127.65
2	B	631	CPR	C6-N1-C2	3.89	121.41	115.84
2	A	631	CPR	C6-N1-C2	3.86	121.37	115.84
3	A	701	NAD	C3D-C2D-C1D	3.27	105.90	100.98
3	B	702	NAD	C3D-C2D-C1D	3.24	105.85	100.98
3	A	701	NAD	C3N-C7N-N7N	-3.15	113.96	117.75
3	A	701	NAD	PN-O3-PA	-2.88	122.94	132.83
3	B	702	NAD	PN-O3-PA	-2.83	123.10	132.83
3	A	701	NAD	C6N-N1N-C2N	-2.80	119.42	121.97
3	B	702	NAD	C3B-C2B-C1B	2.64	104.96	100.98
3	B	702	NAD	C6N-N1N-C2N	-2.63	119.58	121.97
3	A	701	NAD	C3B-C2B-C1B	2.56	104.84	100.98
3	A	701	NAD	O7N-C7N-C3N	2.40	122.50	119.63
2	B	631	CPR	O2P-P-O1P	2.03	118.64	110.68
2	A	631	CPR	O2P-P-O1P	2.03	118.63	110.68
3	B	702	NAD	O7N-C7N-C3N	2.01	122.04	119.63

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	C5B-O5B-PA-O3
3	A	701	NAD	C5D-O5D-PN-O3
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	C5B-O5B-PA-O3
3	B	702	NAD	C5D-O5D-PN-O3
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	C5D-O5D-PN-O2N
3	B	702	NAD	C5B-O5B-PA-O1A
3	B	702	NAD	C5B-O5B-PA-O2A
3	B	702	NAD	C5D-O5D-PN-O2N
3	A	701	NAD	PN-O3-PA-O1A
3	B	702	NAD	PN-O3-PA-O1A
3	A	701	NAD	C2D-C1D-N1N-C2N
3	B	702	NAD	C2D-C1D-N1N-C2N
3	A	701	NAD	PN-O3-PA-O2A
3	B	702	NAD	PN-O3-PA-O2A

There are no ring outliers.

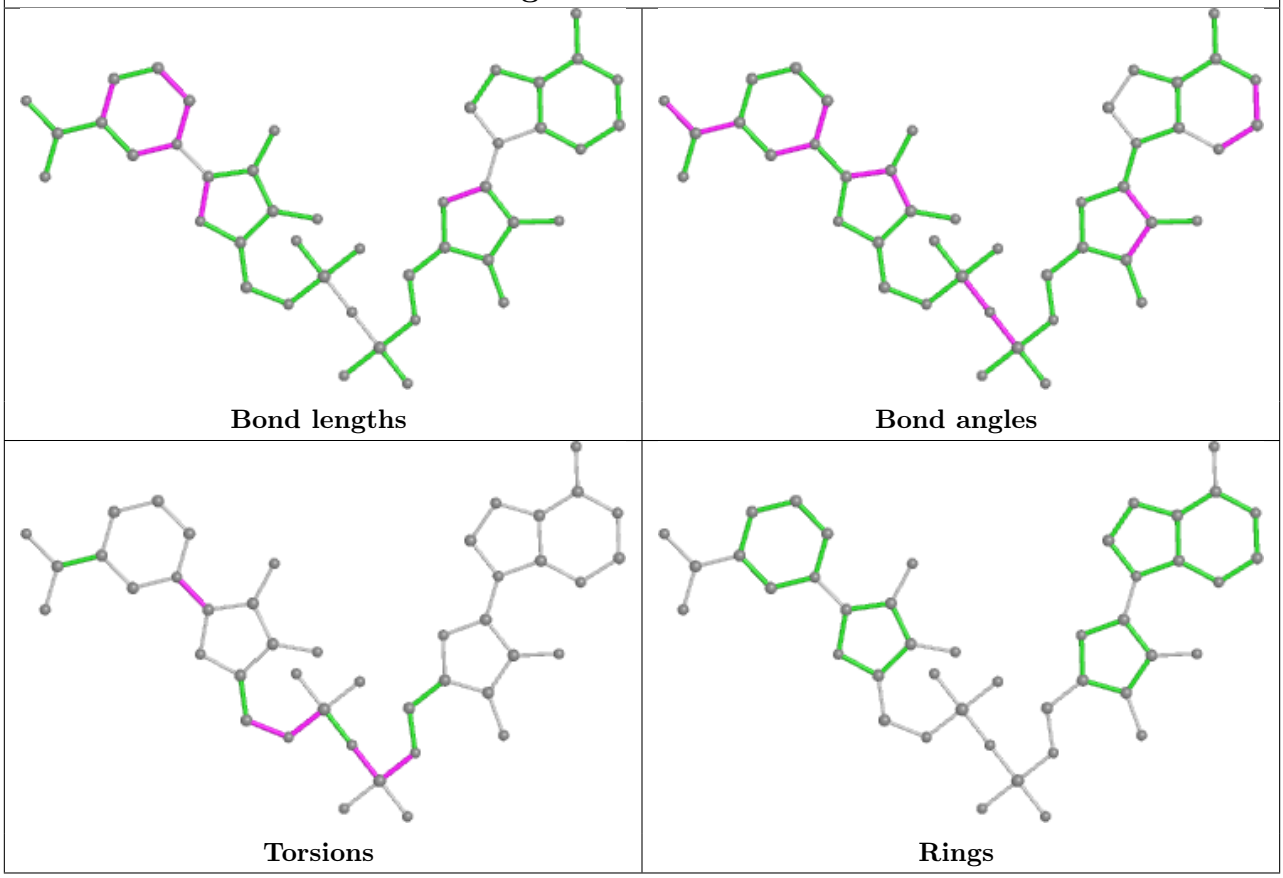
4 monomers are involved in 14 short contacts:

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

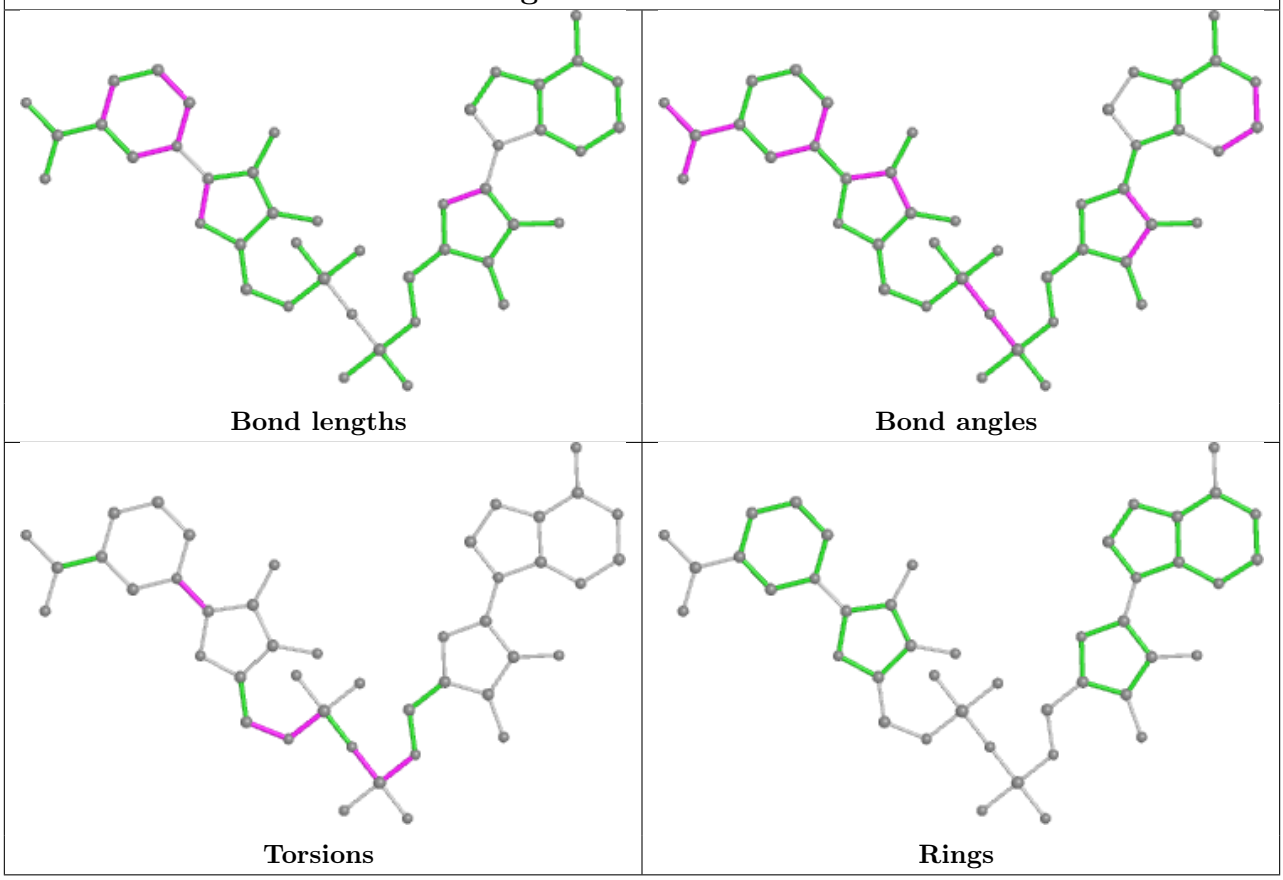
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

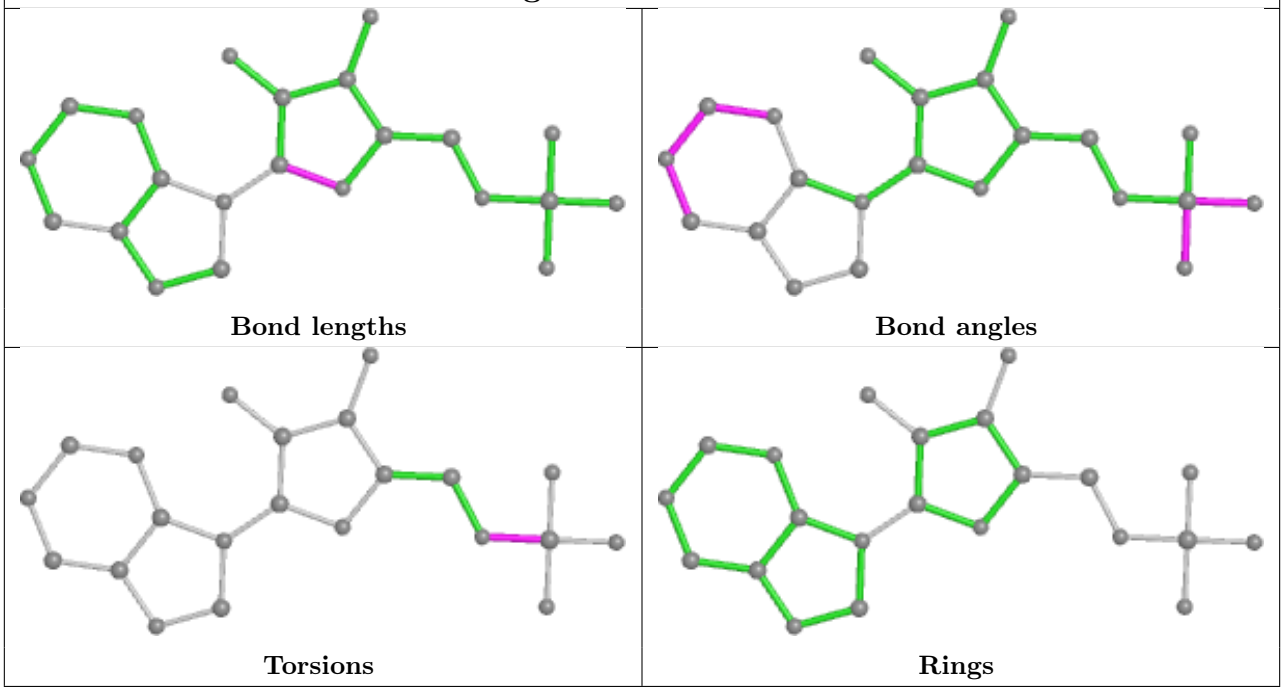
Ligand NAD B 702



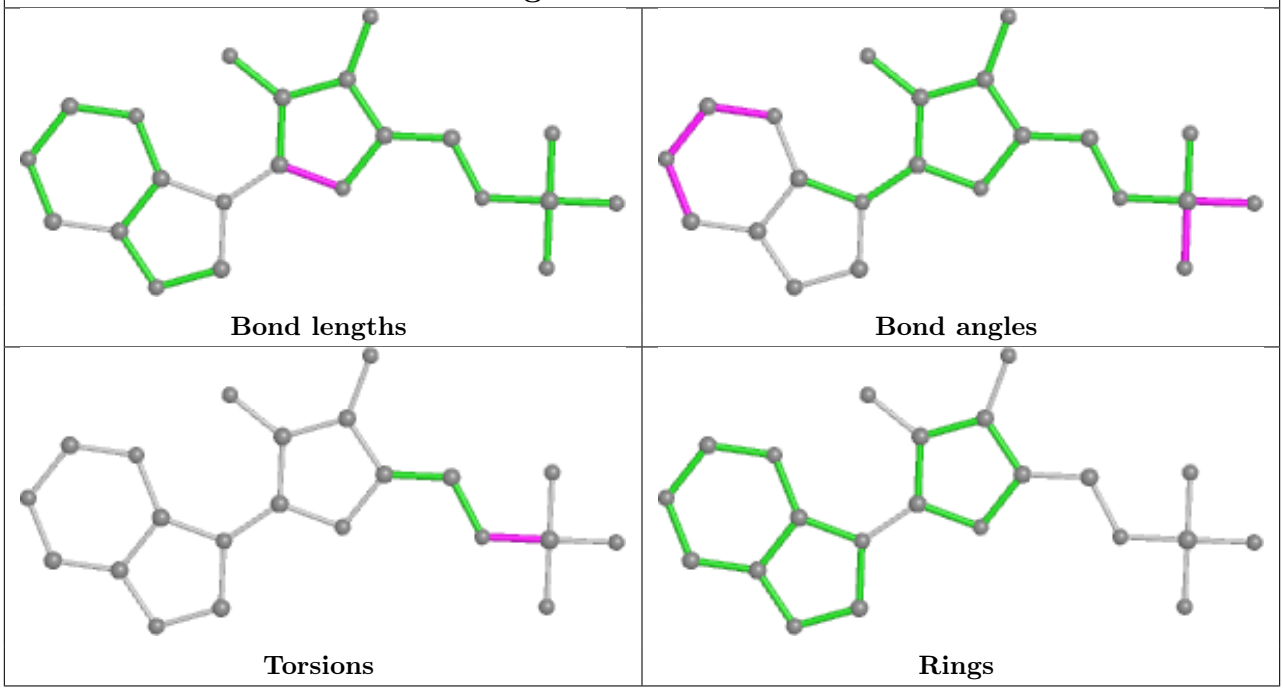
Ligand NAD A 701



Ligand CPR A 631



Ligand CPR B 631



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%)	0.67	40 (10%)	7	5	18, 52, 110, 143	0
1	B	396/514 (77%)	0.70	39 (9%)	7	5	17, 52, 112, 148	0
All	All	792/1028 (77%)	0.68	79 (9%)	7	5	17, 52, 111, 148	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	411	TYR	13.8
1	A	411	TYR	12.7
1	B	403	SER	12.2
1	B	413	GLY	10.7
1	B	402	PHE	10.6
1	B	122	SER	9.9
1	A	141	GLY	8.5
1	A	191	GLY	8.2
1	A	414	MET	7.7
1	A	333	THR	7.7
1	A	402	PHE	7.3
1	A	403	SER	7.1
1	B	412	ARG	7.1
1	A	413	GLY	7.1
1	B	406	ILE	6.8
1	A	334	GLN	6.8
1	A	152	SER	6.7
1	B	207	GLY	6.6
1	A	401	PHE	6.3
1	B	335	GLU	6.2
1	A	400	TYR	6.2
1	B	141	GLY	6.0
1	B	333	THR	5.9
1	B	408	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	122	SER	5.6
1	B	404	ASP	5.1
1	B	230	ASN	5.1
1	A	223	ALA	5.1
1	A	123	PRO	5.0
1	A	207	GLY	5.0
1	B	405	GLY	4.8
1	B	334	GLN	4.4
1	A	212	VAL	4.3
1	A	213	ASN	4.2
1	A	335	GLU	4.2
1	B	216	ASP	4.2
1	B	496	SER	4.1
1	B	142	ILE	4.1
1	B	152	SER	4.0
1	A	412	ARG	4.0
1	B	123	PRO	3.9
1	B	191	GLY	3.8
1	A	192	ILE	3.8
1	B	401	PHE	3.8
1	A	230	ASN	3.7
1	B	198	ASN	3.6
1	B	414	MET	3.6
1	B	498	GLN	3.5
1	A	142	ILE	3.3
1	A	188	ALA	3.2
1	B	337	LEU	3.2
1	A	496	SER	3.1
1	A	410	LYS	3.1
1	B	197	ALA	3.0
1	B	407	ARG	3.0
1	B	399	GLU	2.9
1	A	197	ALA	2.9
1	B	400	TYR	2.8
1	A	406	ILE	2.7
1	B	215	ASP	2.7
1	A	409	LYS	2.6
1	B	188	ALA	2.6
1	A	151	GLY	2.6
1	A	114	PHE	2.5
1	A	399	GLU	2.5
1	A	404	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	146	ASP	2.4
1	B	120	VAL	2.3
1	A	343	GLN	2.3
1	B	336	VAL	2.2
1	A	405	GLY	2.2
1	A	121	LEU	2.1
1	A	407	ARG	2.1
1	B	189	PRO	2.1
1	B	151	GLY	2.1
1	A	216	ASP	2.1
1	B	190	ALA	2.0
1	A	120	VAL	2.0
1	A	498	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

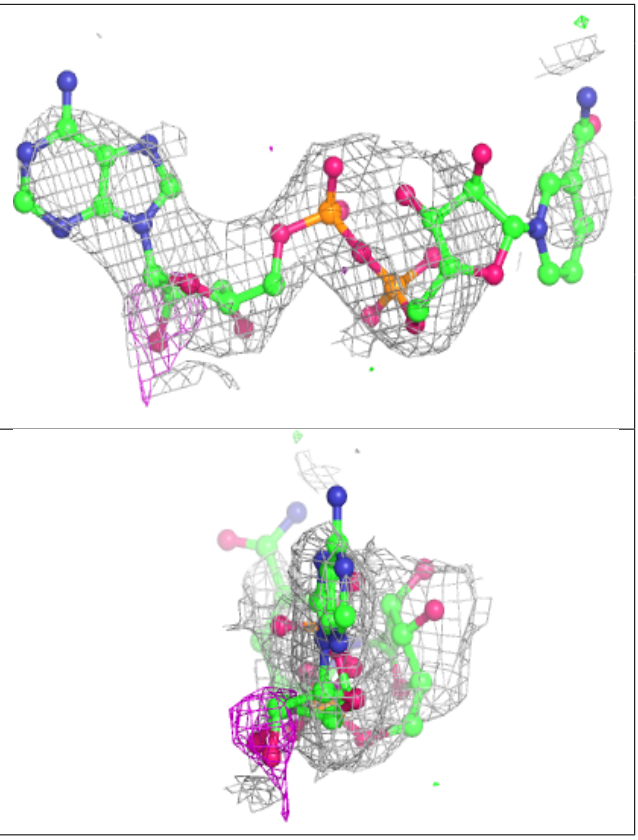
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	702	44/44	0.77	0.44	138,138,138,138	0
3	NAD	A	701	44/44	0.82	0.36	126,126,126,126	0
2	CPR	A	631	22/23	0.93	0.23	74,75,75,76	0
2	CPR	B	631	22/23	0.93	0.19	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.

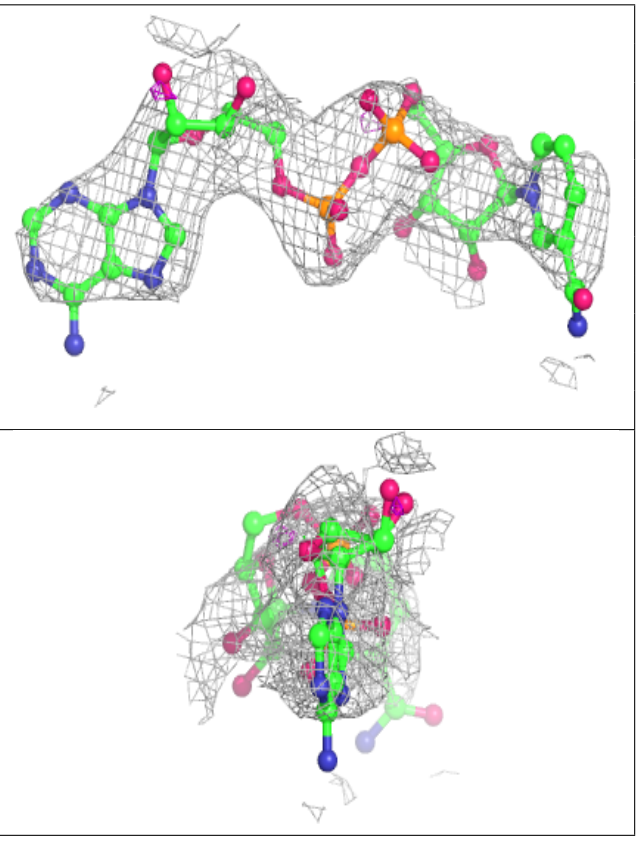
Electron density around NAD B 702:

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



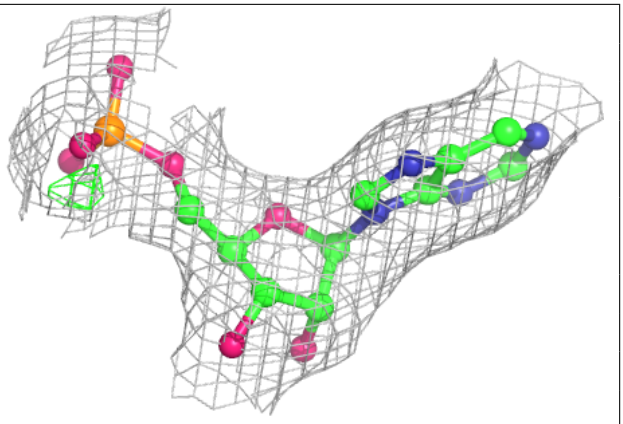
Electron density around NAD A 701:

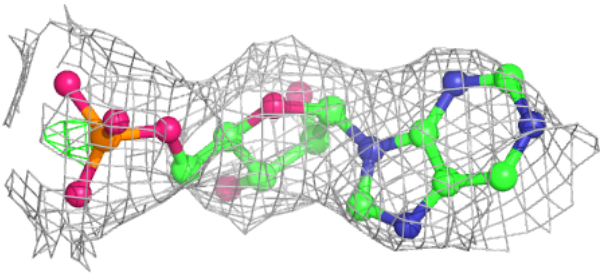
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

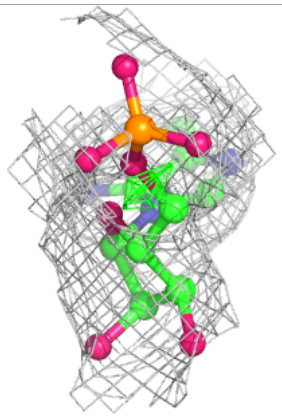


Electron density around CPR A 631:

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

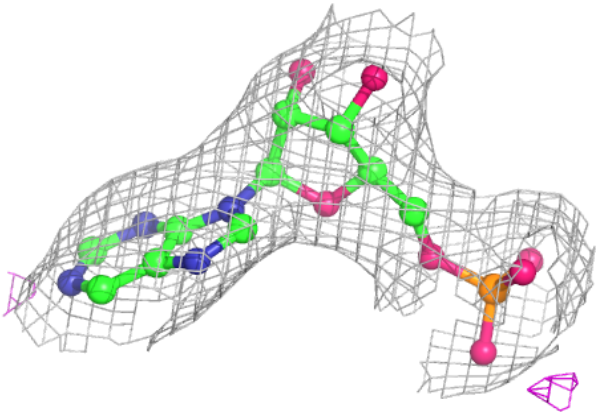


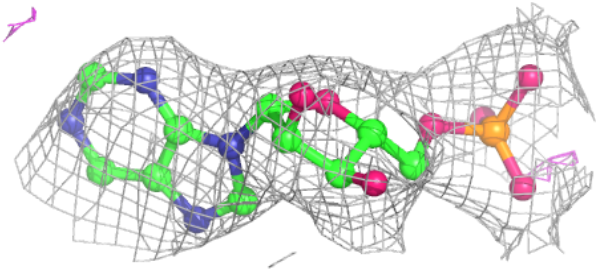


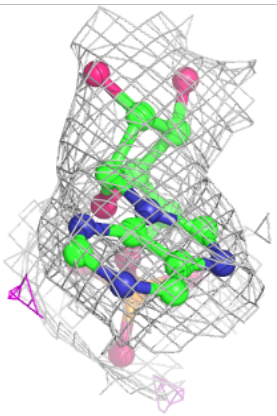


Electron density around CPR B 631:

$2mF_o$-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 (i)

There are no such residues in this entry.