Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:59 AM EDT

PDB ID	:	1P1I
Title	:	Crystal structure of the NAD+-bound 1L-myo-inositol 1-phosphate synthase
Authors	:	Jin, X.; Geiger, J.H.
Deposited on	:	2003-04-12
Resolution	:	2.40 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:

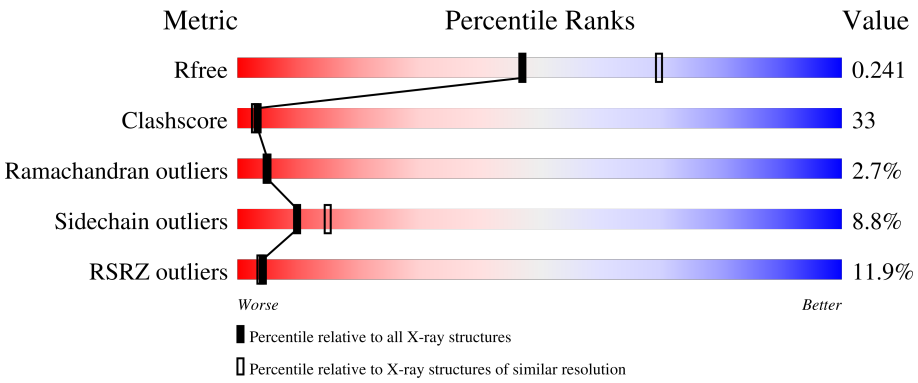
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	533	10% 49% 41% 5% 5%
1	B	533	13% 43% 44% 6% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8163 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 Inositol-3-phosphate synthase.

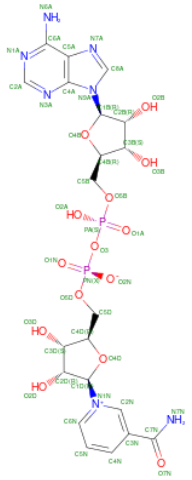
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	506	3989	2539	668	766	16	0	0	0
1	B	498	3926	2502	658	750	16	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	SEE REMARK 999	UNP P11986
A	14	VAL	LEU	SEE REMARK 999	UNP P11986
A	?	-	PHE	SEE REMARK 999	UNP P11986
A	60	LEU	GLU	SEE REMARK 999	UNP P11986
A	?	-	ALA	SEE REMARK 999	UNP P11986
A	98	GLU	LYS	SEE REMARK 999	UNP P11986
A	140	ASN	LYS	SEE REMARK 999	UNP P11986
A	141	ASP	HIS	SEE REMARK 999	UNP P11986
A	201	ASN	GLN	SEE REMARK 999	UNP P11986
A	444	PRO	ALA	SEE REMARK 999	UNP P11986
B	?	-	ARG	SEE REMARK 999	UNP P11986
B	14	VAL	LEU	SEE REMARK 999	UNP P11986
B	?	-	PHE	SEE REMARK 999	UNP P11986
B	60	LEU	GLU	SEE REMARK 999	UNP P11986
B	?	-	ALA	SEE REMARK 999	UNP P11986
B	98	GLU	LYS	SEE REMARK 999	UNP P11986
B	140	ASN	LYS	SEE REMARK 999	UNP P11986
B	141	ASP	HIS	SEE REMARK 999	UNP P11986
B	201	ASN	GLN	SEE REMARK 999	UNP P11986
B	444	PRO	ALA	SEE REMARK 999	UNP P11986

- Molecule 2 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		
2	A	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
2	B	1	44	21	7	14	2	0	0

- Molecule 3 is water.

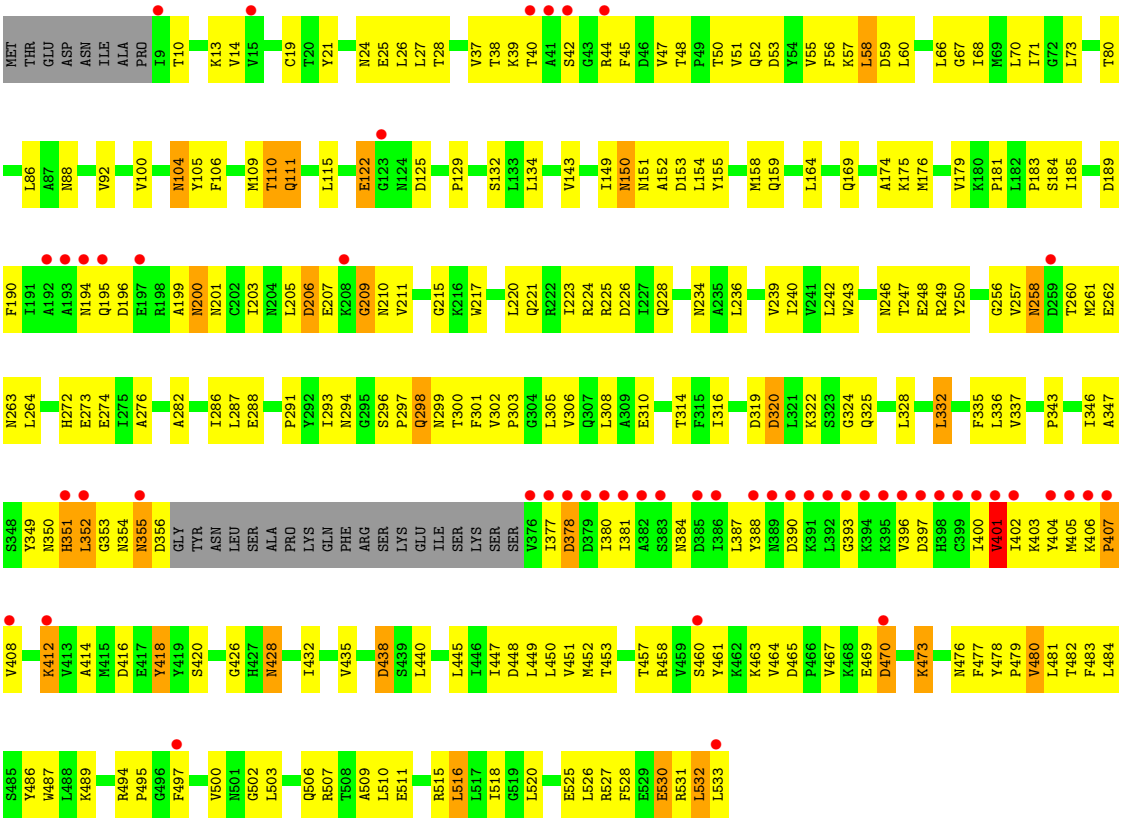
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	90	90	90	0	0
			Total	O		
3	B	70	70	70	0	0

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.

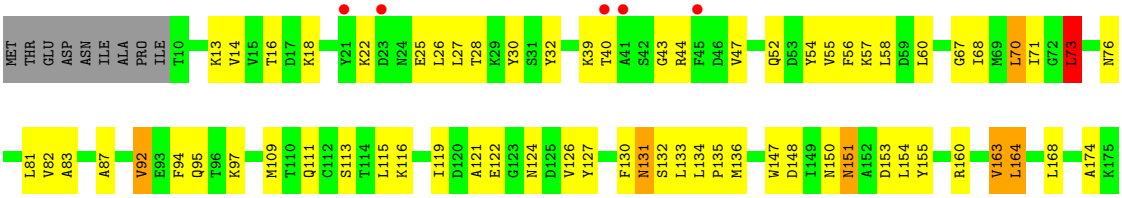
• Molecule 1: Inositol-3-phosphate synthase

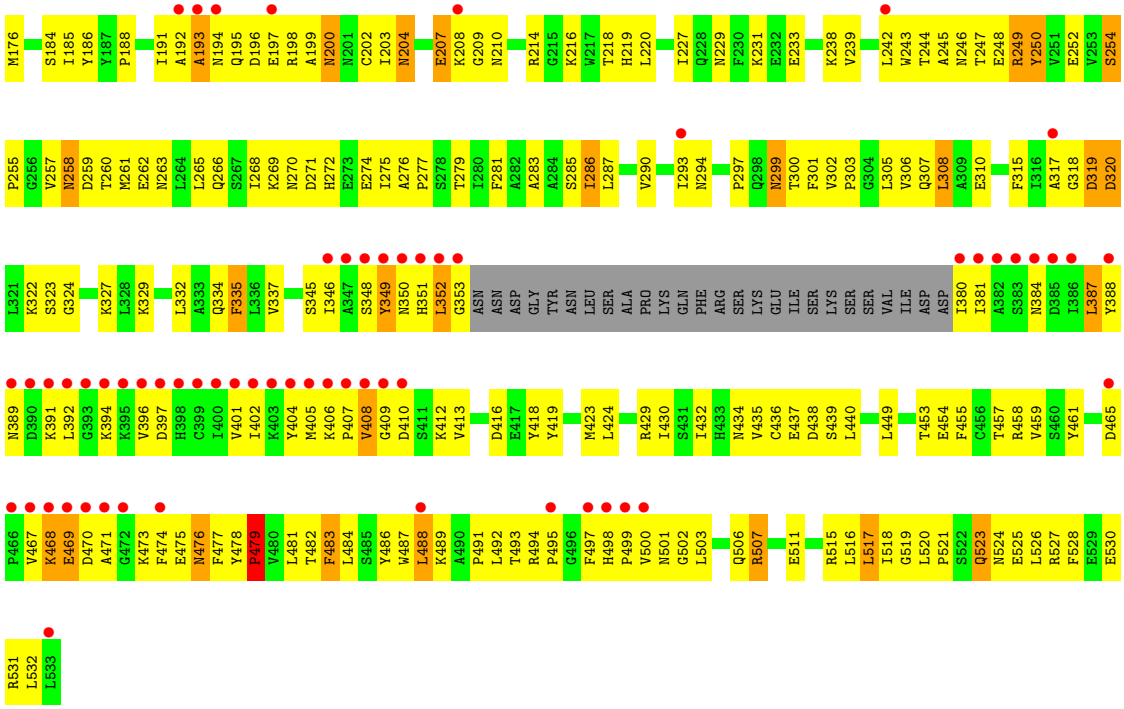
Chain A:



• Molecule 1: Inositol-3-phosphate synthase

Chain B:




M176 S184 I185 Y186 Y187 P188 I191 A192 A193 N194 Q195 D196 E197 R198 A199 N200 N201 C202 I203 N204 E207 K208 G209 N210 R214 G215 K216 W217 T218 H219 L220 I227 Q228 N229 F230 K231 E232 E233 K238 V239 L242 W243 T244 A245 N246 T247 E248 R249 Y250 V251 E252 V253 S254
P255 G256 V257 N258 D259 T260 M261 E262 N263 L264 L265 Q266 S267 I268 K269 N270 D271 H272 E273 E274 I275 A276 P277 S278 T279 I280 F281 A282 A283 A284 S285 I286 L287 V290 I293 N294 P297 Q298 N299 T300 F301 V302 P303 G304 L305 V306 Q307 L308 A309 E310 F315 I316 A317 G318 D319 D320
L321 K322 S323 G324 K327 L328 K329 L332 A333 Q334 F335 L336 V337 S345 I346 A347 S348 Y349 N350 H351 L352 G353 ASN ASN ASP GLY TYR ASN LEU SER ALA PRO LYS GLN PHE ARG SER LYS GLU ILE SER LYS SER SER VAL ILE ASP ASP I380 I381 A382 S383 N384 D385 I386 L387 Y388
N389 D390 K391 L392 G393 K394 K395 V396 D397 H398 C399 I400 V401 I402 K403 Y404 M405 K406 P407 V408 G409 D410 S411 K412 V413 D416 E417 Y418 Y419 M423 L424 R429 I430 S431 I432 H433 N434 V435 C436 E437 D438 S439 L440 L449 T453 E454 F455 C456 T457 R458 V459 S460 Y461 D465
P466 V467 K468 E469 D470 A471 G472 K473 F474 E475 N476 F477 Y478 P479 Y480 L481 T482 F483 L484 S485 Y486 W487 L488 K489 A490 P491 L492 T493 R494 P495 G496 F497 H498 P499 V500 N501 G502 L503 Q506 R507 E511 R515 L516 L517 I518 G519 L520 P521 S522 Q523 N524 E525 L526 R527 F528 E529 E530
R531 L532 L533

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.38Å 97.34Å 122.89Å 90.00° 126.53° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 32.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.40) 99.4 (32.92-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.288 0.246 , 0.241	Depositor DCC
R_{free} test set	2857 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 70.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8163	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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

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	0.39	0/4066	0.65	0/5514
1	B	0.39	0/4003	0.65	2/5427 (0.0%)
All	All	0.39	0/8069	0.65	2/10941 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	73	LEU	CA-CB-CG	5.34	127.58	115.30
1	B	319	ASP	N-CA-C	5.28	125.25	111.00

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	3989	0	3994	263	0
1	B	3926	0	3939	303	0
2	A	44	0	26	2	0
2	B	44	0	26	5	0
3	A	90	0	0	6	0
3	B	70	0	0	5	0
All	All	8163	0	7985	525	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 33.

All (525) 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:332:LEU:HD13	1:B:432:ILE:HD11	1.24	1.11
1:A:246:ASN:HD22	2:A:650:NAD:H8A	1.23	1.03
1:B:286:ILE:HD12	1:B:308:LEU:HD13	1.45	0.98
1:B:293:ILE:HA	1:B:317:ALA:HB2	1.49	0.93
1:A:110:THR:HB	1:A:448:ASP:OD1	1.71	0.91
1:B:476:ASN:H	1:B:476:ASN:HD22	1.15	0.90
1:A:104:ASN:ND2	1:A:106:PHE:H	1.69	0.90
1:A:509:ALA:HB1	1:B:531:ARG:HH12	1.38	0.89
1:B:254:SER:H	1:B:258:ASN:HD21	1.22	0.88
1:A:531:ARG:HD3	1:B:482:THR:OG1	1.73	0.87
1:A:353:GLY:HA2	1:A:406:LYS:HA	1.56	0.86
1:A:13:LYS:HE3	1:B:44:ARG:NH1	1.92	0.84
1:A:110:THR:HG22	1:A:111:GLN:NE2	1.93	0.84
1:B:87:ALA:HA	1:B:92:VAL:CG1	2.07	0.84
1:B:468:LYS:HZ2	1:B:471:ALA:HB1	1.41	0.83
1:A:68:ILE:HD12	1:A:450:LEU:HD13	1.61	0.83
1:A:325:GLN:NE2	1:A:350:ASN:HD21	1.76	0.83
1:B:293:ILE:HA	1:B:317:ALA:CB	2.07	0.83
1:A:257:VAL:HG11	1:A:274:GLU:OE2	1.79	0.82
1:B:87:ALA:HA	1:B:92:VAL:HG13	1.62	0.82
1:B:324:GLY:HA2	1:B:327:LYS:HD3	1.62	0.81
1:A:37:VAL:HG11	1:B:126:VAL:HG11	1.61	0.81
1:A:104:ASN:HD22	1:A:106:PHE:H	1.27	0.81
1:B:58:LEU:HD23	1:B:459:VAL:HG22	1.64	0.80
1:A:449:LEU:O	1:A:453:THR:HG23	1.81	0.80
1:B:349:TYR:HB3	1:B:401:VAL:HB	1.64	0.79
1:B:381:ILE:HG23	1:B:388:TYR:HB3	1.65	0.79
1:A:412:LYS:HZ2	1:A:412:LYS:HB3	1.46	0.79
1:B:476:ASN:H	1:B:476:ASN:ND2	1.81	0.77
1:A:502:GLY:O	1:A:506:GLN:HG3	1.84	0.76
1:A:13:LYS:HE3	1:B:44:ARG:HH12	1.48	0.76
1:A:158:MET:HE1	1:A:176:MET:HG3	1.68	0.75
1:B:238:LYS:NZ	1:B:457:THR:HG21	2.01	0.75
1:B:115:LEU:HD22	1:B:511:GLU:HG3	1.67	0.75
1:B:135:PRO:HG2	1:B:458:ARG:HH22	1.51	0.75
1:B:286:ILE:HD11	1:B:308:LEU:HD22	1.68	0.74
1:A:352:LEU:HD12	1:A:354:ASN:OD1	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ILE:CD1	1:B:308:LEU:HD13	2.17	0.73
1:A:13:LYS:CE	1:B:44:ARG:HH12	2.01	0.73
1:B:109:MET:O	1:B:113:SER:HB3	1.87	0.73
1:B:523:GLN:HA	1:B:523:GLN:HE21	1.53	0.73
1:A:332:LEU:HG	1:A:432:ILE:HD11	1.70	0.73
1:B:52:GLN:HG3	1:B:54:TYR:CE1	2.24	0.73
1:B:286:ILE:HD13	1:B:287:LEU:N	2.04	0.72
1:B:468:LYS:NZ	1:B:471:ALA:HB1	2.05	0.72
1:A:310:GLU:HA	1:A:479:PRO:HG2	1.72	0.71
1:B:492:LEU:HD13	1:B:493:THR:N	2.06	0.71
1:A:352:LEU:HD23	1:A:352:LEU:H	1.53	0.71
1:B:384:ASN:HD21	1:B:387:LEU:HD22	1.55	0.71
1:B:135:PRO:HG2	1:B:458:ARG:NH2	2.04	0.71
1:B:150:ASN:HD21	1:B:160:ARG:HH12	1.38	0.71
1:B:476:ASN:HD22	1:B:476:ASN:N	1.84	0.71
1:A:110:THR:HG22	1:A:111:GLN:HE21	1.55	0.70
1:B:406:LYS:HB3	1:B:407:PRO:HD3	1.73	0.70
1:B:109:MET:HE1	1:B:507:ARG:NH2	2.06	0.70
1:B:410:ASP:OD2	1:B:437:GLU:HB3	1.91	0.70
1:A:104:ASN:HD21	1:B:423:MET:HA	1.56	0.70
1:A:453:THR:O	1:A:457:THR:HG23	1.92	0.70
1:A:533:LEU:HA	1:B:494:ARG:HH22	1.55	0.70
1:A:150:ASN:ND2	1:A:152:ALA:H	1.89	0.69
1:B:254:SER:N	1:B:258:ASN:HD21	1.90	0.69
1:B:261:MET:O	1:B:265:LEU:HD13	1.91	0.69
1:B:302:VAL:O	1:B:306:VAL:HG23	1.93	0.69
1:A:44:ARG:HH21	1:B:13:LYS:HG2	1.58	0.68
1:A:224:ARG:O	1:A:228:GLN:HG3	1.93	0.68
1:A:353:GLY:CA	1:A:406:LYS:HA	2.23	0.68
1:B:294:ASN:H	1:B:317:ALA:HB3	1.58	0.68
1:B:131:ASN:HD22	1:B:132:SER:N	1.93	0.67
1:B:454:GLU:O	1:B:457:THR:HB	1.93	0.67
1:B:345:SER:HB3	1:B:419:TYR:HB3	1.76	0.67
1:B:25:GLU:OE1	1:B:57:LYS:HD3	1.93	0.67
1:A:272:HIS:CD2	1:A:274:GLU:HB2	2.29	0.67
1:A:400:ILE:HG22	1:A:401:VAL:H	1.58	0.67
1:A:473:LYS:H	1:A:473:LYS:HD2	1.60	0.67
1:B:109:MET:HE1	1:B:507:ARG:HG3	1.77	0.67
1:A:352:LEU:HD23	1:A:352:LEU:N	2.09	0.66
1:B:473:LYS:HD2	1:B:474:PHE:H	1.60	0.66
1:B:516:LEU:HD12	1:B:517:LEU:N	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ASN:ND2	1:B:387:LEU:HD22	2.10	0.66
1:A:246:ASN:ND2	2:A:650:NAD:H8A	2.05	0.66
1:A:328:LEU:HD21	1:B:430:ILE:HG21	1.78	0.66
1:B:507:ARG:HG3	1:B:507:ARG:HH21	1.60	0.65
1:B:227:ILE:O	1:B:231:LYS:HG3	1.96	0.65
1:B:58:LEU:HD23	1:B:459:VAL:CG2	2.24	0.65
1:B:492:LEU:HD13	1:B:493:THR:H	1.61	0.65
1:B:258:ASN:HD22	1:B:258:ASN:H	1.44	0.65
1:B:404:TYR:HE1	1:B:406:LYS:HB2	1.62	0.65
1:B:334:GLN:HA	1:B:380:ILE:HD13	1.78	0.65
1:B:57:LYS:HE3	1:B:474:PHE:CD2	2.33	0.64
1:A:200:ASN:H	1:A:200:ASN:HD22	1.45	0.64
1:A:478:TYR:CE1	1:A:494:ARG:HB3	2.32	0.64
1:A:350:ASN:HB2	1:A:402:ILE:HA	1.78	0.64
1:A:481:LEU:HB3	1:A:484:LEU:CD2	2.28	0.64
1:B:203:ILE:HG13	1:B:204:ASN:N	2.13	0.64
1:A:478:TYR:CD2	1:A:479:PRO:HD2	2.32	0.64
1:B:478:TYR:CD1	1:B:479:PRO:HD2	2.33	0.64
1:A:37:VAL:CG1	1:B:126:VAL:HG11	2.27	0.63
1:B:247:THR:CG2	1:B:297:PRO:HG2	2.28	0.63
1:A:104:ASN:HD22	1:A:105:TYR:N	1.96	0.63
1:A:190:PHE:O	1:A:248:GLU:HA	1.98	0.63
1:B:121:ALA:HB3	1:B:122:GLU:OE2	1.97	0.63
1:B:329:LYS:HG3	1:B:418:TYR:OH	1.98	0.63
1:A:195:GLN:HE22	1:A:355:ASN:HD21	1.48	0.62
1:B:277:PRO:HG2	3:B:665:HOH:O	1.99	0.62
1:B:387:LEU:HA	1:B:392:LEU:HD22	1.80	0.62
1:B:249:ARG:HG2	1:B:249:ARG:HH21	1.65	0.62
1:B:216:LYS:HA	1:B:219:HIS:CD2	2.35	0.62
1:A:481:LEU:HB3	1:A:484:LEU:HD23	1.81	0.62
1:B:299:ASN:HD22	1:B:299:ASN:N	1.97	0.62
1:B:493:THR:HG21	1:B:499:PRO:HD3	1.82	0.62
1:A:149:ILE:O	1:A:199:ALA:HA	1.99	0.62
1:B:30:TYR:CE1	1:B:32:TYR:HB2	2.35	0.61
1:B:40:THR:HG23	1:B:44:ARG:O	1.99	0.61
1:B:352:LEU:N	1:B:352:LEU:HD23	2.15	0.61
1:B:261:MET:H	1:B:307:GLN:NE2	1.99	0.61
1:B:515:ARG:NH1	1:B:521:PRO:O	2.33	0.61
1:A:14:VAL:HA	1:B:47:VAL:HG13	1.81	0.61
1:B:57:LYS:HB2	1:B:474:PHE:CE2	2.35	0.61
1:A:400:ILE:O	1:A:401:VAL:HG23	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ARG:HB2	1:A:531:ARG:NH2	2.15	0.61
1:B:56:PHE:CD2	1:B:461:TYR:HB3	2.34	0.61
1:B:302:VAL:HB	1:B:303:PRO:HD2	1.83	0.61
1:A:21:TYR:CE1	1:A:26:LEU:HD13	2.36	0.61
1:B:14:VAL:HG11	1:B:518:ILE:O	2.01	0.61
1:B:151:ASN:H	1:B:200:ASN:HD21	1.47	0.61
1:B:315:PHE:CD1	1:B:481:LEU:HD11	2.36	0.60
1:A:381:ILE:HG13	1:A:388:TYR:CG	2.36	0.60
1:A:486:TYR:HA	1:A:506:GLN:OE1	2.01	0.60
1:A:150:ASN:HD22	1:A:152:ALA:H	1.48	0.60
1:A:404:TYR:CE2	1:A:406:LYS:HB2	2.37	0.60
1:B:185:ILE:HG12	1:B:203:ILE:HD11	1.84	0.60
1:B:58:LEU:CD1	1:B:60:LEU:HD23	2.31	0.60
1:A:206:ASP:OD1	1:A:210:ASN:HB2	2.02	0.60
1:A:217:TRP:O	1:A:221:GLN:HG2	2.01	0.60
1:A:272:HIS:CD2	1:A:274:GLU:H	2.20	0.60
1:B:381:ILE:HG23	1:B:388:TYR:CB	2.32	0.59
1:A:405:MET:O	1:A:408:VAL:HG22	2.01	0.59
1:A:19:CYS:HB3	1:A:28:THR:OG1	2.03	0.59
1:B:469:GLU:HG2	1:B:470:ASP:N	2.17	0.59
1:A:316:ILE:HD11	1:A:480:VAL:HG22	1.82	0.59
1:A:500:VAL:HG21	1:B:527:ARG:CZ	2.33	0.59
1:A:350:ASN:O	1:A:351:HIS:HB3	2.02	0.59
1:A:509:ALA:CB	1:B:531:ARG:HH12	2.13	0.59
1:B:349:TYR:CB	1:B:401:VAL:HB	2.31	0.59
1:A:158:MET:CE	1:A:176:MET:HG3	2.32	0.59
1:A:38:THR:HG22	1:A:39:LYS:N	2.18	0.59
1:A:294:ASN:ND2	1:A:296:SER:H	2.01	0.58
1:B:352:LEU:HD21	1:B:402:ILE:HD11	1.86	0.58
1:A:14:VAL:HG21	1:A:518:ILE:HD12	1.85	0.58
1:A:516:LEU:C	1:A:516:LEU:HD23	2.24	0.58
1:B:299:ASN:HD22	1:B:299:ASN:H	1.52	0.58
1:A:185:ILE:HG12	1:A:203:ILE:HD11	1.86	0.57
1:B:200:ASN:C	1:B:200:ASN:ND2	2.58	0.57
1:A:205:LEU:HD13	1:A:209:GLY:HA2	1.85	0.57
1:A:92:VAL:HG12	1:A:92:VAL:O	2.04	0.57
1:A:297:PRO:HB3	1:A:320:ASP:OD2	2.04	0.57
1:B:134:LEU:HD21	1:B:518:ILE:CG2	2.34	0.57
1:B:255:PRO:HA	1:B:259:ASP:CG	2.25	0.57
1:A:44:ARG:NH2	1:B:13:LYS:HG2	2.20	0.57
1:B:58:LEU:HD12	1:B:60:LEU:HD23	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:HD13	1:B:478:TYR:HD1	1.69	0.57
1:B:249:ARG:HD2	1:B:250:TYR:O	2.05	0.57
1:B:332:LEU:HD13	1:B:432:ILE:CD1	2.16	0.57
1:B:348:SER:HB3	1:B:416:ASP:OD1	2.04	0.57
1:B:192:ALA:O	1:B:194:ASN:N	2.38	0.56
1:B:26:LEU:O	1:B:57:LYS:HA	2.04	0.56
1:B:489:LYS:O	1:B:491:PRO:HD3	2.05	0.56
1:A:125:ASP:CG	1:A:527:ARG:HH22	2.07	0.56
1:B:97:LYS:HB2	1:B:97:LYS:NZ	2.20	0.56
1:B:134:LEU:HD12	1:B:455:PHE:HZ	1.70	0.56
1:A:388:TYR:HA	1:A:393:GLY:O	2.05	0.56
1:B:73:LEU:HD13	1:B:154:LEU:HD11	1.85	0.56
1:A:52:GLN:NE2	1:A:463:LYS:HD2	2.21	0.56
1:B:109:MET:HE1	1:B:507:ARG:HH21	1.69	0.56
1:B:528:PHE:O	1:B:532:LEU:HB2	2.04	0.56
1:A:406:LYS:O	1:A:408:VAL:N	2.34	0.56
1:B:131:ASN:HD22	1:B:132:SER:H	1.52	0.56
1:B:30:TYR:HE1	1:B:32:TYR:HB2	1.71	0.56
1:B:310:GLU:HG2	1:B:479:PRO:HG2	1.87	0.56
1:A:494:ARG:HB2	1:A:495:PRO:HD2	1.88	0.55
1:A:37:VAL:HG22	1:A:47:VAL:HG22	1.86	0.55
1:B:192:ALA:O	1:B:195:GLN:N	2.40	0.55
1:B:476:ASN:ND2	1:B:476:ASN:N	2.47	0.55
1:A:200:ASN:HD22	1:A:200:ASN:N	2.02	0.55
1:B:238:LYS:HZ1	1:B:457:THR:HG21	1.71	0.55
1:A:39:LYS:HA	1:A:44:ARG:O	2.05	0.55
1:A:406:LYS:HD3	1:A:406:LYS:C	2.25	0.55
1:B:323:SER:HB3	1:B:489:LYS:HZ1	1.71	0.55
1:B:220:LEU:C	1:B:220:LEU:HD23	2.27	0.55
1:B:500:VAL:HG12	1:B:502:GLY:H	1.70	0.55
1:A:13:LYS:NZ	1:B:44:ARG:HH12	2.04	0.55
1:B:468:LYS:NZ	1:B:471:ALA:CB	2.69	0.55
1:A:381:ILE:HD12	1:A:396:VAL:HG23	1.89	0.55
1:B:391:LYS:HB2	1:B:391:LYS:HZ2	1.71	0.55
1:A:272:HIS:HD2	1:A:274:GLU:HB2	1.72	0.54
1:A:325:GLN:HE22	1:A:350:ASN:HD21	1.50	0.54
1:A:205:LEU:HB3	1:A:209:GLY:HA2	1.89	0.54
1:B:404:TYR:CE1	1:B:406:LYS:HB2	2.42	0.54
1:A:377:ILE:O	1:A:381:ILE:HG22	2.07	0.54
1:B:332:LEU:HD23	1:B:332:LEU:C	2.28	0.54
1:A:302:VAL:O	1:A:306:VAL:HG23	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:THR:HG21	1:B:297:PRO:HG2	1.90	0.54
1:A:412:LYS:O	1:A:435:VAL:HA	2.07	0.54
1:A:528:PHE:CD1	1:A:532:LEU:HD22	2.43	0.54
1:B:247:THR:HG23	1:B:297:PRO:HG2	1.90	0.54
1:B:150:ASN:ND2	1:B:160:ARG:HH12	2.03	0.54
1:B:320:ASP:OD2	2:B:660:NAD:H6N	2.08	0.54
1:A:68:ILE:HG22	1:A:70:LEU:HD13	1.90	0.54
1:B:200:ASN:C	1:B:200:ASN:HD22	2.09	0.54
1:B:255:PRO:HA	1:B:259:ASP:OD1	2.08	0.54
1:A:39:LYS:HD2	1:A:44:ARG:O	2.08	0.54
1:A:412:LYS:HZ1	1:A:414:ALA:HB2	1.74	0.53
1:B:95:GLN:HA	1:B:95:GLN:NE2	2.23	0.53
1:B:272:HIS:CE1	1:B:274:GLU:HB2	2.43	0.53
1:A:402:ILE:HD13	3:A:737:HOH:O	2.07	0.53
1:B:516:LEU:HD12	1:B:516:LEU:C	2.29	0.53
1:A:406:LYS:O	1:A:406:LYS:HD3	2.08	0.53
1:A:350:ASN:N	1:A:401:VAL:O	2.42	0.53
1:B:468:LYS:HG2	1:B:471:ALA:HB2	1.90	0.53
1:A:287:LEU:HD21	1:A:308:LEU:HD11	1.91	0.53
1:A:322:LYS:HD3	1:A:503:LEU:HD13	1.89	0.53
1:B:16:THR:HG21	1:B:519:GLY:HA3	1.91	0.53
1:A:58:LEU:HD13	1:A:60:LEU:HD12	1.91	0.52
1:B:244:THR:HG23	1:B:244:THR:O	2.08	0.52
1:B:283:ALA:HA	1:B:286:ILE:HG23	1.91	0.52
1:A:282:ALA:O	1:A:286:ILE:HG13	2.08	0.52
1:A:353:GLY:O	1:A:406:LYS:HG2	2.08	0.52
1:A:150:ASN:HD22	1:A:151:ASN:N	2.06	0.52
1:A:38:THR:HG22	1:A:39:LYS:H	1.74	0.52
1:A:509:ALA:HB1	1:B:531:ARG:NH1	2.17	0.52
1:A:14:VAL:CG2	1:A:518:ILE:HD12	2.39	0.52
1:A:150:ASN:HA	1:A:200:ASN:ND2	2.24	0.52
1:A:190:PHE:CE2	1:A:276:ALA:HB2	2.44	0.52
1:A:258:ASN:H	1:A:258:ASN:ND2	2.08	0.52
1:B:208:LYS:C	1:B:210:ASN:H	2.13	0.52
1:A:378:ASP:HA	1:A:381:ILE:HG22	1.91	0.52
1:A:40:THR:HB	1:A:44:ARG:HB3	1.91	0.51
1:A:473:LYS:H	1:A:473:LYS:CD	2.23	0.51
1:B:238:LYS:HZ2	1:B:457:THR:HG21	1.75	0.51
1:B:484:LEU:O	1:B:488:LEU:HD22	2.10	0.51
1:B:381:ILE:HD11	1:B:396:VAL:HG23	1.92	0.51
1:A:418:TYR:OH	1:A:432:ILE:HD12	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ASN:ND2	1:B:391:LYS:HB3	2.25	0.51
1:A:164:LEU:N	1:A:164:LEU:HD12	2.25	0.51
1:B:299:ASN:H	1:B:299:ASN:ND2	2.07	0.51
1:A:105:TYR:HA	1:B:423:MET:HE3	1.93	0.51
1:A:528:PHE:C	1:A:530:GLU:H	2.14	0.51
1:B:322:LYS:HA	1:B:489:LYS:HG3	1.93	0.51
1:B:134:LEU:HD21	1:B:518:ILE:HG22	1.93	0.51
1:A:273:GLU:HB2	3:A:722:HOH:O	2.11	0.50
1:B:28:THR:O	1:B:55:VAL:HA	2.11	0.50
1:B:207:GLU:C	1:B:209:GLY:H	2.13	0.50
1:B:523:GLN:HE21	1:B:523:GLN:CA	2.18	0.50
1:A:150:ASN:HA	1:A:200:ASN:HD21	1.75	0.50
1:A:484:LEU:HD22	1:A:484:LEU:N	2.27	0.50
1:B:67:GLY:O	1:B:68:ILE:HD13	2.11	0.50
1:B:306:VAL:O	1:B:310:GLU:HG3	2.11	0.50
1:B:467:VAL:O	1:B:468:LYS:HB2	2.12	0.50
1:A:256:GLY:C	1:A:263:ASN:HD22	2.15	0.50
1:A:445:LEU:HD21	1:A:487:TRP:HB3	1.94	0.50
1:B:134:LEU:HB3	1:B:135:PRO:HD2	1.93	0.50
1:A:469:GLU:HG2	1:A:470:ASP:N	2.26	0.50
1:A:258:ASN:H	1:A:258:ASN:HD22	1.58	0.50
1:B:95:GLN:HE21	1:B:95:GLN:CA	2.25	0.50
1:B:97:LYS:NZ	1:B:97:LYS:CB	2.75	0.50
1:B:122:GLU:CD	1:B:122:GLU:H	2.15	0.50
1:A:88:ASN:HD21	1:A:104:ASN:HA	1.76	0.49
1:A:100:VAL:O	1:A:100:VAL:HG13	2.11	0.49
1:A:150:ASN:HD22	1:A:150:ASN:C	2.15	0.49
1:A:426:GLY:HA3	1:B:440:LEU:CD1	2.42	0.49
1:B:285:SER:O	1:B:290:VAL:HG22	2.12	0.49
1:A:435:VAL:HG13	1:B:429:ARG:HB3	1.94	0.49
1:B:332:LEU:CD1	1:B:432:ILE:HD11	2.17	0.49
1:B:389:ASN:HD21	1:B:391:LYS:HB3	1.77	0.49
1:A:426:GLY:HA3	1:B:440:LEU:HD13	1.94	0.49
1:B:258:ASN:HD22	1:B:258:ASN:N	2.03	0.49
1:B:413:VAL:HA	1:B:434:ASN:O	2.12	0.49
1:A:264:LEU:HD22	1:A:305:LEU:HA	1.93	0.49
1:B:337:VAL:HG21	1:B:380:ILE:HG22	1.95	0.49
1:A:384:ASN:CG	1:A:387:LEU:HD12	2.33	0.49
1:A:104:ASN:HD22	1:A:106:PHE:N	2.03	0.49
1:A:478:TYR:HE1	1:A:494:ARG:HB3	1.77	0.49
1:B:350:ASN:HD21	1:B:402:ILE:HG13	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:MET:O	1:B:408:VAL:HG23	2.12	0.49
1:B:252:GLU:O	1:B:274:GLU:OE1	2.29	0.49
1:B:381:ILE:HD11	1:B:396:VAL:CG2	2.43	0.49
1:B:337:VAL:HG21	1:B:380:ILE:CG2	2.43	0.49
1:A:347:ALA:HB1	1:A:349:TYR:CE2	2.48	0.49
1:B:348:SER:CB	1:B:416:ASP:HA	2.43	0.49
1:A:335:PHE:HZ	1:B:327:LYS:HE2	1.77	0.48
1:A:343:PRO:HA	1:A:420:SER:HA	1.94	0.48
1:A:351:HIS:HA	1:A:403:LYS:O	2.12	0.48
1:B:192:ALA:C	1:B:194:ASN:H	2.16	0.48
1:B:218:THR:HG23	3:B:699:HOH:O	2.12	0.48
1:B:249:ARG:HG2	1:B:249:ARG:NH2	2.27	0.48
1:A:24:ASN:O	1:A:60:LEU:HB2	2.12	0.48
1:B:219:HIS:HE1	3:B:697:HOH:O	1.95	0.48
1:B:449:LEU:HD21	1:B:487:TRP:HB2	1.96	0.48
1:A:143:VAL:HG21	1:A:236:LEU:HD21	1.96	0.48
1:B:318:GLY:HA2	1:B:492:LEU:HB2	1.94	0.48
1:B:412:LYS:O	1:B:435:VAL:HA	2.12	0.48
1:B:523:GLN:HA	1:B:523:GLN:NE2	2.24	0.48
1:A:200:ASN:N	1:A:200:ASN:ND2	2.62	0.48
1:A:234:ASN:HB2	1:A:236:LEU:HG	1.95	0.48
1:A:400:ILE:HG22	1:A:401:VAL:N	2.27	0.48
1:B:286:ILE:HD13	1:B:286:ILE:C	2.34	0.48
1:B:352:LEU:HB3	1:B:412:LYS:HG3	1.95	0.48
1:B:39:LYS:HG3	1:B:43:GLY:HA2	1.96	0.48
1:B:147:TRP:CD2	1:B:281:PHE:HE2	2.31	0.48
1:A:19:CYS:HA	1:A:27:LEU:O	2.13	0.48
1:A:50:THR:HG22	3:A:677:HOH:O	2.14	0.48
1:B:195:GLN:HE22	1:B:198:ARG:HD2	1.79	0.48
1:A:56:PHE:CE1	1:A:461:TYR:HB3	2.49	0.47
1:A:481:LEU:HD13	1:A:484:LEU:HD21	1.95	0.47
1:B:131:ASN:HD22	1:B:131:ASN:N	2.12	0.47
1:B:82:VAL:HG21	1:B:154:LEU:CD2	2.44	0.47
1:A:19:CYS:HB3	1:A:28:THR:HA	1.96	0.47
1:A:412:LYS:HB3	1:A:412:LYS:NZ	2.25	0.47
1:A:511:GLU:O	1:A:515:ARG:HG3	2.14	0.47
1:A:533:LEU:CD1	1:B:478:TYR:HD1	2.27	0.47
1:B:18:LYS:O	1:B:28:THR:HA	2.14	0.47
1:A:247:THR:CG2	1:A:297:PRO:HG2	2.45	0.47
1:A:406:LYS:HB3	1:A:407:PRO:HD3	1.97	0.47
1:A:445:LEU:C	1:A:445:LEU:HD23	2.34	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ARG:HD3	1:B:482:THR:HG1	1.73	0.47
1:A:533:LEU:HD22	1:A:533:LEU:H	1.79	0.47
1:B:193:ALA:C	1:B:195:GLN:H	2.18	0.47
1:B:229:ASN:O	1:B:233:GLU:HB3	2.14	0.47
1:A:155:TYR:O	1:A:159:GLN:HG3	2.14	0.47
1:B:208:LYS:CB	1:B:210:ASN:HD22	2.28	0.47
1:A:67:GLY:HA3	1:A:239:VAL:HG22	1.96	0.47
1:A:88:ASN:HD21	1:A:104:ASN:CA	2.28	0.47
1:A:154:LEU:HD22	1:A:179:VAL:CG1	2.44	0.47
1:B:453:THR:HG23	1:B:481:LEU:CD1	2.44	0.47
1:A:220:LEU:O	1:A:224:ARG:HG3	2.15	0.47
1:B:26:LEU:HB2	1:B:60:LEU:HD21	1.96	0.47
1:B:300:THR:O	1:B:302:VAL:N	2.45	0.47
1:A:412:LYS:NZ	1:A:414:ALA:HB2	2.29	0.47
1:B:293:ILE:HG23	1:B:317:ALA:CB	2.45	0.47
1:B:26:LEU:HD12	1:B:27:LEU:H	1.79	0.46
1:A:497:PHE:CE2	1:B:530:GLU:HB2	2.50	0.46
1:B:266:GLN:HE21	1:B:270:ASN:HD21	1.63	0.46
1:B:270:ASN:O	1:B:271:ASP:HB2	2.15	0.46
1:B:524:ASN:O	1:B:525:GLU:HB2	2.14	0.46
1:B:95:GLN:HA	1:B:95:GLN:HE21	1.80	0.46
1:A:350:ASN:HD22	1:A:412:LYS:HE2	1.80	0.46
1:A:428:ASN:ND2	1:B:436:CYS:HB3	2.30	0.46
1:B:153:ASP:OD2	1:B:155:TYR:N	2.42	0.46
1:B:353:GLY:HA3	1:B:409:GLY:O	2.16	0.46
1:A:378:ASP:HA	1:A:381:ILE:CG2	2.46	0.46
1:B:258:ASN:N	1:B:258:ASN:ND2	2.63	0.46
1:A:153:ASP:OD2	1:A:153:ASP:C	2.54	0.46
1:A:256:GLY:HA2	1:A:263:ASN:ND2	2.31	0.46
1:B:380:ILE:HG22	1:B:380:ILE:O	2.16	0.46
1:A:286:ILE:HA	1:A:314:THR:HG21	1.96	0.45
1:B:76:ASN:HB3	1:B:439:SER:OG	2.16	0.45
1:B:134:LEU:HB3	1:B:135:PRO:CD	2.47	0.45
1:B:122:GLU:CD	1:B:122:GLU:N	2.70	0.45
1:B:131:ASN:N	1:B:131:ASN:ND2	2.64	0.45
1:A:14:VAL:HG22	1:B:47:VAL:CG1	2.47	0.45
1:A:55:VAL:HG23	1:A:464:VAL:HG21	1.99	0.45
1:B:97:LYS:HB2	1:B:97:LYS:HZ2	1.80	0.45
1:B:465:ASP:OD2	1:B:467:VAL:HB	2.16	0.45
1:A:223:ILE:O	1:A:226:ASP:HB2	2.17	0.45
1:A:258:ASN:ND2	1:A:258:ASN:N	2.62	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:PHE:CZ	1:B:327:LYS:HE2	2.51	0.45
1:B:186:TYR:CZ	1:B:188:PRO:HB3	2.52	0.45
1:B:192:ALA:C	1:B:194:ASN:N	2.68	0.45
1:B:389:ASN:OD1	1:B:392:LEU:HD13	2.17	0.45
1:A:44:ARG:HH21	1:B:13:LYS:CG	2.27	0.45
1:A:337:VAL:HG21	1:A:380:ILE:HG22	1.98	0.45
1:B:130:PHE:CE2	1:B:136:MET:HE1	2.51	0.45
1:B:200:ASN:HD22	1:B:200:ASN:H	1.65	0.45
1:B:391:LYS:HB2	1:B:391:LYS:NZ	2.32	0.45
1:A:122:GLU:OE2	1:A:122:GLU:N	2.50	0.45
1:A:352:LEU:N	1:A:352:LEU:CD2	2.79	0.45
1:A:183:PRO:HB2	1:A:203:ILE:HG23	2.00	0.44
1:A:325:GLN:HG3	3:A:652:HOH:O	2.16	0.44
1:B:150:ASN:ND2	1:B:160:ARG:NH1	2.64	0.44
1:A:115:LEU:HD22	1:A:511:GLU:HB3	2.00	0.44
1:A:286:ILE:HG23	1:A:314:THR:HB	1.98	0.44
1:A:378:ASP:CA	1:A:381:ILE:HG22	2.47	0.44
1:B:83:ALA:HB2	1:B:176:MET:HE2	1.99	0.44
1:A:351:HIS:O	1:A:351:HIS:ND1	2.51	0.44
1:B:285:SER:HB3	1:B:290:VAL:HG23	1.99	0.44
1:B:302:VAL:HG23	1:B:305:LEU:H	1.82	0.44
1:A:301:PHE:HA	1:A:305:LEU:HD23	1.98	0.44
1:B:26:LEU:HD12	1:B:27:LEU:N	2.33	0.44
1:B:272:HIS:ND1	1:B:274:GLU:N	2.59	0.44
1:B:352:LEU:N	1:B:352:LEU:CD2	2.81	0.44
1:A:465:ASP:OD1	1:A:467:VAL:HG22	2.18	0.44
1:B:293:ILE:CA	1:B:317:ALA:HB2	2.35	0.44
1:A:57:LYS:HB3	1:A:460:SER:HB3	1.98	0.44
1:A:169:GLN:HE21	1:A:169:GLN:HB3	1.61	0.44
1:A:500:VAL:HG21	1:B:527:ARG:NH2	2.32	0.44
1:B:246:ASN:HD22	2:B:660:NAD:H8A	1.81	0.44
1:B:438:ASP:HB3	2:B:660:NAD:O7N	2.18	0.44
1:B:174:ALA:HB3	3:B:669:HOH:O	2.18	0.44
1:B:293:ILE:HA	1:B:317:ALA:HB3	1.93	0.44
1:A:52:GLN:OE1	1:A:53:ASP:O	2.36	0.44
1:B:259:ASP:OD2	1:B:259:ASP:N	2.49	0.44
1:B:348:SER:OG	1:B:416:ASP:HA	2.18	0.44
1:B:350:ASN:O	1:B:351:HIS:HB3	2.18	0.44
1:A:109:MET:HE2	1:A:507:ARG:HE	1.83	0.43
1:A:302:VAL:HB	1:A:303:PRO:HD2	2.00	0.43
1:A:530:GLU:HG3	1:B:497:PHE:HD2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:SER:H	1:B:258:ASN:ND2	2.03	0.43
1:B:468:LYS:HG2	1:B:471:ALA:CB	2.48	0.43
1:A:104:ASN:HD22	1:A:104:ASN:C	2.21	0.43
1:A:184:SER:OG	1:A:185:ILE:N	2.49	0.43
1:B:94:PHE:CD2	1:B:94:PHE:N	2.86	0.43
1:A:440:LEU:HD12	1:A:440:LEU:HA	1.83	0.43
1:A:447:ILE:O	1:A:451:VAL:HG23	2.19	0.43
1:A:520:LEU:HA	1:A:520:LEU:HD23	1.77	0.43
1:A:525:GLU:HA	1:A:525:GLU:OE2	2.18	0.43
1:A:532:LEU:HG	1:B:461:TYR:CZ	2.54	0.43
1:B:254:SER:O	1:B:257:VAL:HG13	2.18	0.43
1:A:38:THR:O	1:A:45:PHE:HA	2.19	0.43
1:A:51:VAL:HG12	1:A:52:GLN:N	2.34	0.43
1:A:47:VAL:HG11	1:B:520:LEU:HD11	2.01	0.43
1:A:125:ASP:OD1	1:A:527:ARG:NH2	2.51	0.43
1:A:134:LEU:HD21	1:A:518:ILE:CG2	2.48	0.43
1:A:190:PHE:HB3	1:A:248:GLU:HB3	2.01	0.43
1:B:260:THR:OG1	1:B:263:ASN:ND2	2.52	0.43
1:A:234:ASN:CB	1:A:236:LEU:HG	2.49	0.43
1:A:354:ASN:HD21	1:A:356:ASP:HB2	1.83	0.43
1:B:115:LEU:O	1:B:127:TYR:HA	2.19	0.43
1:B:276:ALA:O	1:B:279:THR:HB	2.19	0.42
1:B:350:ASN:HD21	1:B:402:ILE:CG1	2.32	0.42
1:B:526:LEU:O	1:B:527:ARG:C	2.57	0.42
1:A:14:VAL:HG22	1:B:47:VAL:HG11	2.00	0.42
1:A:533:LEU:HD22	1:A:533:LEU:N	2.34	0.42
1:B:184:SER:OG	1:B:185:ILE:N	2.52	0.42
1:B:381:ILE:HG23	1:B:388:TYR:CG	2.54	0.42
1:A:349:TYR:HD1	1:A:401:VAL:HB	1.84	0.42
1:A:476:ASN:O	1:A:477:PHE:C	2.58	0.42
1:A:483:PHE:CE1	1:B:531:ARG:HD3	2.55	0.42
1:B:163:VAL:HG23	1:B:164:LEU:HD13	2.01	0.42
1:B:350:ASN:ND2	1:B:402:ILE:HG13	2.35	0.42
1:B:501:ASN:HA	1:B:506:GLN:OE1	2.19	0.42
1:A:10:THR:HG21	1:A:129:PRO:HG2	2.00	0.42
1:A:242:LEU:HD12	1:A:293:ILE:HD12	2.01	0.42
1:A:247:THR:HG23	1:A:298:GLN:HE21	1.84	0.42
1:A:250:TYR:CD2	1:A:299:ASN:OD1	2.73	0.42
1:B:71:ILE:HG13	1:B:147:TRP:CE3	2.54	0.42
1:B:473:LYS:CD	1:B:474:PHE:H	2.30	0.42
1:A:516:LEU:C	1:A:516:LEU:CD2	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:GLN:NE2	1:B:195:GLN:HA	2.35	0.42
1:B:248:GLU:OE1	1:B:277:PRO:HD2	2.20	0.42
1:B:258:ASN:H	1:B:258:ASN:ND2	2.13	0.42
1:B:384:ASN:ND2	1:B:387:LEU:HB2	2.35	0.42
1:B:525:GLU:OE2	1:B:527:ARG:NH1	2.53	0.42
1:B:265:LEU:O	1:B:269:LYS:HG3	2.19	0.42
1:B:184:SER:O	1:B:202:CYS:HA	2.20	0.42
1:B:185:ILE:CG1	1:B:203:ILE:HD11	2.48	0.42
1:B:322:LYS:NZ	1:B:503:LEU:HD13	2.35	0.42
1:B:493:THR:CG2	1:B:499:PRO:HB3	2.50	0.42
1:A:294:ASN:ND2	1:A:294:ASN:C	2.72	0.42
1:A:19:CYS:CB	1:A:28:THR:OG1	2.67	0.42
1:A:264:LEU:HD21	1:A:305:LEU:HD13	2.00	0.42
1:B:56:PHE:HA	1:B:461:TYR:HA	2.02	0.42
1:A:328:LEU:HD13	1:B:335:PHE:CE1	2.55	0.41
1:A:347:ALA:O	1:A:416:ASP:HA	2.20	0.41
1:B:95:GLN:NE2	1:B:95:GLN:CA	2.83	0.41
1:B:208:LYS:HB2	1:B:210:ASN:HD22	1.85	0.41
1:A:80:THR:HG23	1:A:164:LEU:HD11	2.01	0.41
1:A:129:PRO:HD2	1:A:132:SER:OG	2.20	0.41
1:A:59:ASP:O	1:A:458:ARG:HD2	2.20	0.41
1:B:498:HIS:CD2	1:B:498:HIS:N	2.87	0.41
1:A:73:LEU:HD23	1:A:181:PRO:HB3	2.01	0.41
1:A:412:LYS:HG3	1:A:438:ASP:OD1	2.20	0.41
1:B:71:ILE:HG21	1:B:243:TRP:CZ3	2.56	0.41
1:B:468:LYS:HZ3	1:B:471:ALA:CB	2.34	0.41
1:A:56:PHE:CD1	1:A:461:TYR:HB3	2.55	0.41
1:A:150:ASN:ND2	1:A:151:ASN:N	2.68	0.41
1:A:325:GLN:HE21	1:A:325:GLN:HB3	1.68	0.41
1:B:231:LYS:HG2	1:B:239:VAL:HG21	2.03	0.41
1:B:268:ILE:HG12	1:B:275:ILE:HD12	2.03	0.41
1:A:10:THR:HG23	1:A:132:SER:CB	2.50	0.41
1:A:67:GLY:CA	1:A:236:LEU:HD13	2.50	0.41
1:A:225:ARG:HD2	1:A:225:ARG:HA	1.85	0.41
1:A:240:ILE:HG23	1:A:291:PRO:HB2	2.02	0.41
1:A:533:LEU:HD23	1:B:461:TYR:OH	2.20	0.41
1:B:148:ASP:HA	2:B:660:NAD:N3A	2.35	0.41
1:A:104:ASN:ND2	1:A:104:ASN:C	2.74	0.41
1:B:70:LEU:HD12	1:B:242:LEU:HB3	2.02	0.41
1:A:175:LYS:HA	1:A:175:LYS:HD3	1.83	0.41
1:A:320:ASP:HB3	1:A:489:LYS:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:N	1:A:407:PRO:CD	2.83	0.41
1:A:215:GLY:HA2	3:A:660:HOH:O	2.21	0.41
1:A:328:LEU:HD11	1:B:332:LEU:HG	2.02	0.41
1:B:195:GLN:NE2	1:B:198:ARG:HD2	2.36	0.41
1:B:254:SER:O	1:B:258:ASN:ND2	2.54	0.41
1:B:424:LEU:HA	3:B:702:HOH:O	2.19	0.41
1:B:486:TYR:CE1	1:B:507:ARG:HB2	2.56	0.41
1:A:21:TYR:CZ	1:A:26:LEU:HD13	2.56	0.41
1:A:174:ALA:HB3	3:A:709:HOH:O	2.20	0.41
1:A:247:THR:HG23	1:A:298:GLN:NE2	2.36	0.41
1:A:322:LYS:HD2	1:A:486:TYR:O	2.21	0.41
1:A:354:ASN:HD21	1:A:356:ASP:CB	2.34	0.41
1:A:381:ILE:HG13	1:A:388:TYR:CD2	2.55	0.41
1:A:507:ARG:O	1:A:510:LEU:HB2	2.21	0.41
1:A:532:LEU:HD23	1:B:54:TYR:CE2	2.55	0.41
1:B:119:ILE:HA	1:B:124:ASN:O	2.21	0.41
1:B:323:SER:O	1:B:327:LYS:HG3	2.21	0.41
1:B:349:TYR:CD1	1:B:349:TYR:N	2.88	0.41
1:A:10:THR:HG23	1:A:132:SER:HB2	2.02	0.40
1:A:195:GLN:NE2	1:A:355:ASN:HD21	2.15	0.40
1:A:228:GLN:HG2	1:A:288:GLU:OE1	2.21	0.40
1:A:452:MET:HG3	1:A:487:TRP:HH2	1.86	0.40
1:B:153:ASP:OD2	1:B:155:TYR:HB3	2.22	0.40
1:A:200:ASN:HD22	1:A:200:ASN:C	2.23	0.40
1:A:26:LEU:CB	1:A:60:LEU:HD11	2.52	0.40
1:A:71:ILE:HG21	1:A:243:TRP:CZ3	2.56	0.40
1:B:245:ALA:HA	2:B:660:NAD:H52A	2.02	0.40
1:B:483:PHE:HD2	1:B:483:PHE:HA	1.81	0.40
1:A:418:TYR:CD1	1:A:418:TYR:N	2.90	0.40
1:B:322:LYS:HD2	1:B:489:LYS:HA	2.03	0.40
1:B:477:PHE:O	1:B:478:TYR:C	2.59	0.40
1:B:484:LEU:HA	1:B:487:TRP:CZ3	2.57	0.40
1:B:507:ARG:NH2	1:B:507:ARG:HG3	2.30	0.40
1:A:109:MET:HE2	1:A:507:ARG:NE	2.36	0.40
1:A:482:THR:OG1	1:B:531:ARG:HG2	2.21	0.40
1:A:526:LEU:O	1:A:531:ARG:HG3	2.21	0.40
1:B:208:LYS:HB3	1:B:210:ASN:ND2	2.37	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	502/533 (94%)	431 (86%)	57 (11%)	14 (3%)	5 4
1	B	494/533 (93%)	429 (87%)	52 (10%)	13 (3%)	5 5
All	All	996/1066 (93%)	860 (86%)	109 (11%)	27 (3%)	5 5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	SER
1	B	199	ALA
1	B	319	ASP
1	B	320	ASP
1	B	468	LYS
1	A	194	ASN
1	A	196	ASP
1	A	206	ASP
1	A	209	GLY
1	A	324	GLY
1	A	351	HIS
1	B	133	LEU
1	B	193	ALA
1	B	204	ASN
1	B	301	PHE
1	B	191	ILE
1	A	319	ASP
1	A	407	PRO
1	A	470	ASP
1	B	22	LYS
1	B	495	PRO
1	A	530	GLU
1	B	346	ILE
1	A	346	ILE
1	A	401	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	480	VAL
1	B	479	PRO

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	447/471 (95%)	409 (92%)	38 (8%)	10 16
1	B	439/471 (93%)	399 (91%)	40 (9%)	9 14
All	All	886/942 (94%)	808 (91%)	78 (9%)	10 15

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	48	THR
1	A	58	LEU
1	A	66	LEU
1	A	86	LEU
1	A	104	ASN
1	A	110	THR
1	A	111	GLN
1	A	122	GLU
1	A	150	ASN
1	A	189	ASP
1	A	200	ASN
1	A	201	ASN
1	A	207	GLU
1	A	211	VAL
1	A	249	ARG
1	A	258	ASN
1	A	260	THR
1	A	261	MET
1	A	262	GLU
1	A	298	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	300	THR
1	A	320	ASP
1	A	332	LEU
1	A	336	LEU
1	A	352	LEU
1	A	355	ASN
1	A	378	ASP
1	A	390	ASP
1	A	397	ASP
1	A	401	VAL
1	A	412	LYS
1	A	418	TYR
1	A	428	ASN
1	A	438	ASP
1	A	473	LYS
1	A	516	LEU
1	A	532	LEU
1	B	70	LEU
1	B	73	LEU
1	B	81	LEU
1	B	92	VAL
1	B	111	GLN
1	B	116	LYS
1	B	131	ASN
1	B	151	ASN
1	B	163	VAL
1	B	164	LEU
1	B	168	LEU
1	B	196	ASP
1	B	197	GLU
1	B	200	ASN
1	B	207	GLU
1	B	214	ARG
1	B	249	ARG
1	B	250	TYR
1	B	254	SER
1	B	258	ASN
1	B	262	GLU
1	B	286	ILE
1	B	299	ASN
1	B	308	LEU
1	B	335	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	349	TYR
1	B	352	LEU
1	B	387	LEU
1	B	394	LYS
1	B	397	ASP
1	B	408	VAL
1	B	469	GLU
1	B	475	GLU
1	B	476	ASN
1	B	479	PRO
1	B	483	PHE
1	B	488	LEU
1	B	507	ARG
1	B	517	LEU
1	B	523	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	77	ASN
1	A	88	ASN
1	A	91	ASN
1	A	104	ASN
1	A	111	GLN
1	A	150	ASN
1	A	151	ASN
1	A	162	GLN
1	A	169	GLN
1	A	170	GLN
1	A	200	ASN
1	A	201	ASN
1	A	210	ASN
1	A	228	GLN
1	A	246	ASN
1	A	258	ASN
1	A	263	ASN
1	A	270	ASN
1	A	272	HIS
1	A	294	ASN
1	A	298	GLN
1	A	307	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	325	GLN
1	A	355	ASN
1	A	384	ASN
1	A	428	ASN
1	A	476	ASN
1	A	504	ASN
1	A	512	ASN
1	A	523	GLN
1	B	91	ASN
1	B	95	GLN
1	B	131	ASN
1	B	150	ASN
1	B	151	ASN
1	B	159	GLN
1	B	170	GLN
1	B	195	GLN
1	B	200	ASN
1	B	201	ASN
1	B	210	ASN
1	B	219	HIS
1	B	221	GLN
1	B	228	GLN
1	B	246	ASN
1	B	258	ASN
1	B	263	ASN
1	B	270	ASN
1	B	299	ASN
1	B	307	GLN
1	B	350	ASN
1	B	476	ASN
1	B	506	GLN
1	B	523	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)

2 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	$\#\|Z\| > 2$
2	NAD	A	650	-	42,48,48	2.17	8 (19%)	50,73,73	1.24	9 (18%)
2	NAD	B	660	-	42,48,48	2.40	10 (23%)	50,73,73	1.33	9 (18%)

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
2	NAD	A	650	-	-	3/26/62/62	0/5/5/5
2	NAD	B	660	-	-	7/26/62/62	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	660	NAD	C2N-N1N	8.46	1.44	1.35
2	B	660	NAD	C4N-C3N	7.13	1.50	1.39
2	A	650	NAD	C4N-C3N	6.87	1.49	1.39
2	A	650	NAD	C2N-N1N	6.65	1.42	1.35
2	B	660	NAD	C6N-N1N	4.68	1.46	1.35
2	A	650	NAD	C6N-N1N	4.58	1.45	1.35
2	A	650	NAD	C5N-C4N	4.39	1.46	1.38
2	B	660	NAD	C2A-N1A	4.17	1.41	1.33
2	B	660	NAD	C5N-C4N	4.05	1.45	1.38
2	A	650	NAD	C2A-N1A	4.04	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	660	NAD	O4B-C1B	-3.87	1.35	1.40
2	B	660	NAD	PA-O3	-3.29	1.55	1.59
2	A	650	NAD	PN-O3	2.73	1.62	1.59
2	B	660	NAD	C3N-C7N	2.61	1.54	1.50
2	B	660	NAD	C2N-C3N	2.30	1.42	1.39
2	B	660	NAD	C4A-N3A	2.07	1.38	1.35
2	A	650	NAD	C2A-N3A	2.03	1.35	1.32
2	A	650	NAD	C3N-C7N	2.02	1.53	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	660	NAD	O4B-C1B-N9A	-3.29	104.38	108.75
2	B	660	NAD	C3N-C7N-N7N	3.12	121.58	117.74
2	A	650	NAD	O2A-PA-O3	2.97	115.31	107.27
2	A	650	NAD	C3N-C7N-N7N	2.89	121.30	117.74
2	B	660	NAD	O2A-PA-O3	2.72	114.64	107.27
2	A	650	NAD	C1B-N9A-C4A	-2.70	121.90	126.64
2	B	660	NAD	C6N-N1N-C2N	-2.64	119.63	121.88
2	B	660	NAD	O7N-C7N-N7N	-2.48	119.03	122.62
2	A	650	NAD	O4D-C4D-C3D	2.39	109.89	105.15
2	A	650	NAD	C4A-C5A-N7A	2.32	111.79	109.34
2	B	660	NAD	C4A-C5A-N7A	2.31	111.77	109.34
2	A	650	NAD	O7N-C7N-N7N	-2.28	119.32	122.62
2	B	660	NAD	O3-PN-O1N	-2.22	104.03	110.70
2	A	650	NAD	C5A-C6A-N6A	2.17	123.61	120.31
2	B	660	NAD	O4B-C4B-C5B	-2.13	102.51	109.33
2	B	660	NAD	C4D-O4D-C1D	-2.13	107.97	109.92
2	A	650	NAD	O4B-C1B-N9A	-2.11	105.95	108.75
2	A	650	NAD	O3-PN-O1N	-2.05	104.54	110.70

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	650	NAD	PN-O3-PA-O5B
2	B	660	NAD	C5B-O5B-PA-O1A
2	B	660	NAD	C5B-O5B-PA-O2A
2	B	660	NAD	C5B-O5B-PA-O3
2	A	650	NAD	PA-O3-PN-O1N
2	B	660	NAD	PA-O3-PN-O2N
2	B	660	NAD	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	650	NAD	PA-O3-PN-O2N
2	B	660	NAD	PA-O3-PN-O1N
2	B	660	NAD	C3B-C4B-C5B-O5B

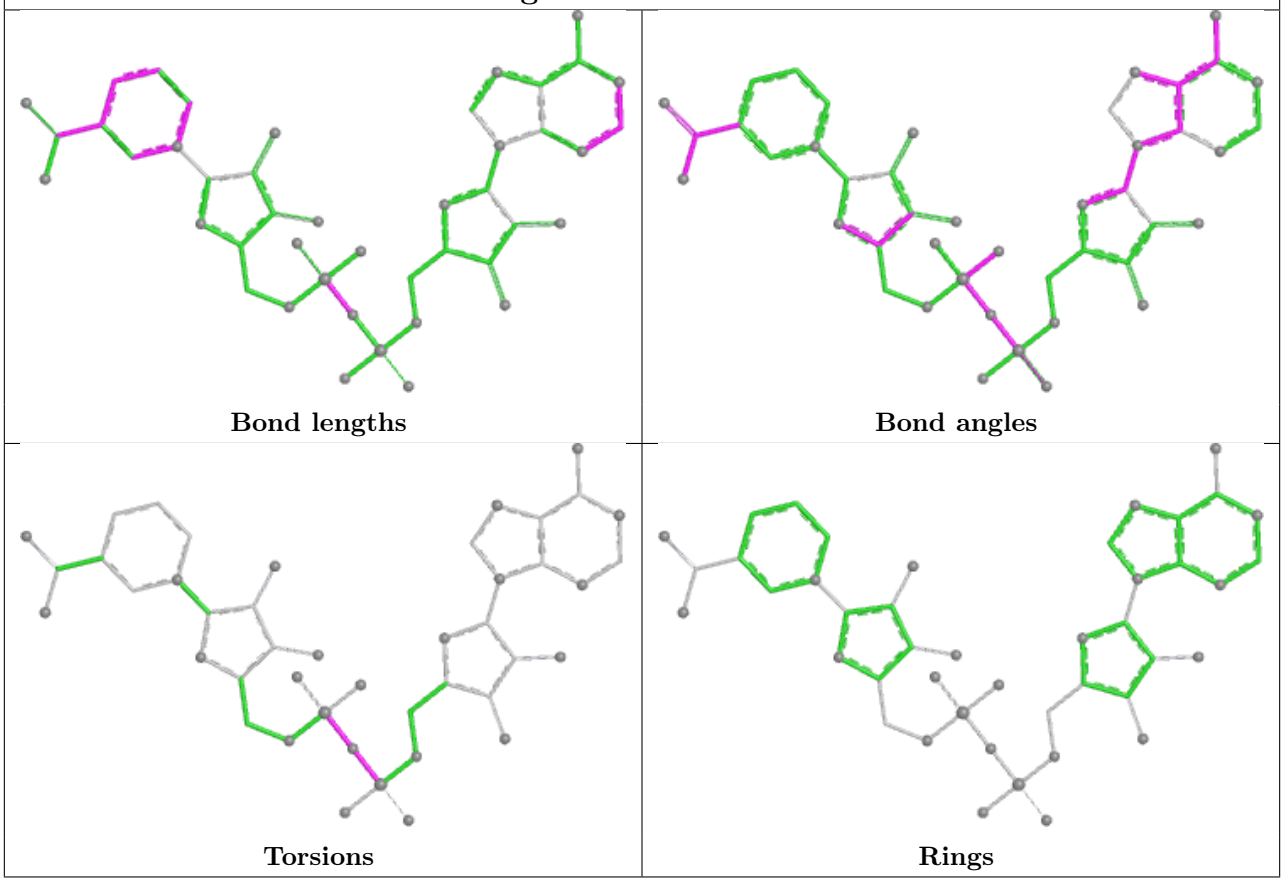
There are no ring outliers.

2 monomers are involved in 7 short contacts:

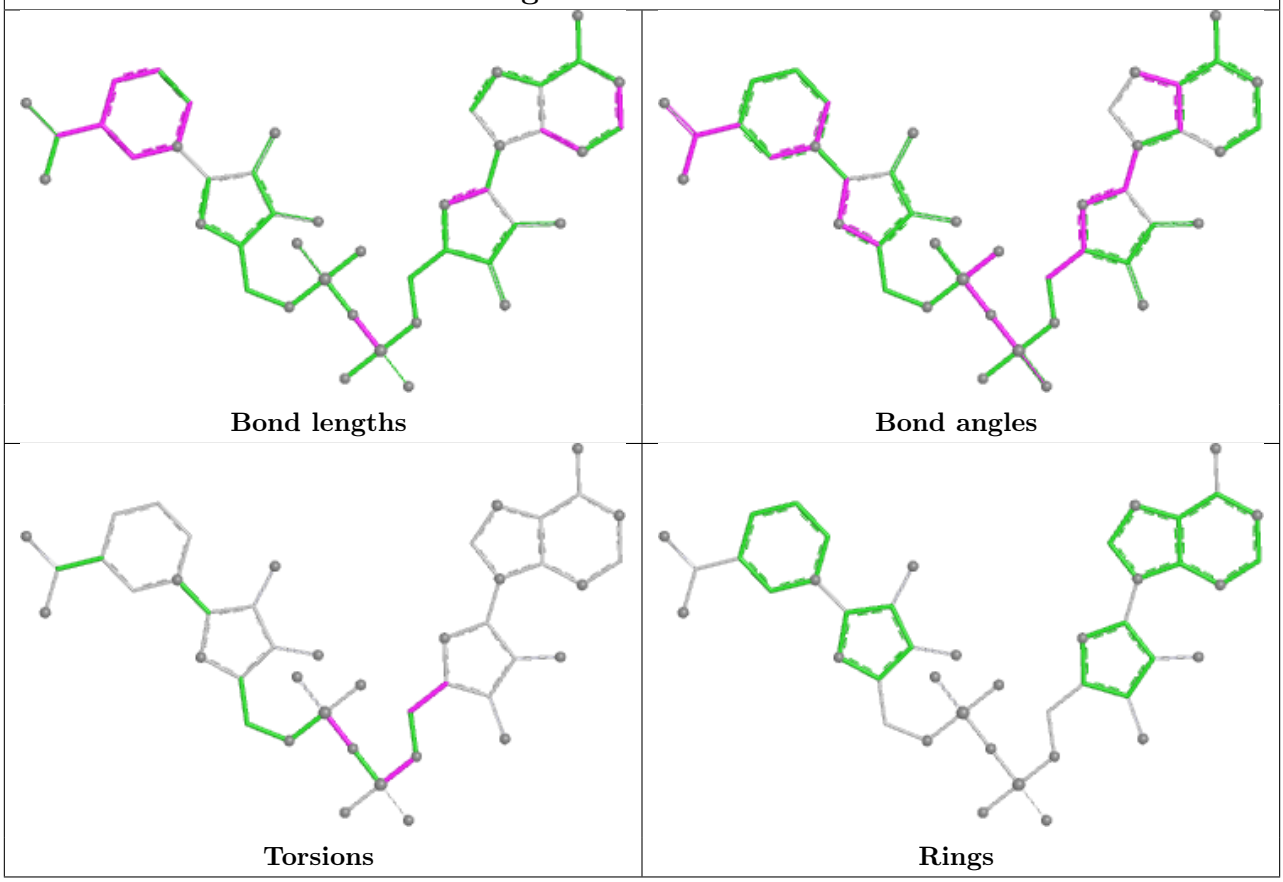
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	650	NAD	2	0
2	B	660	NAD	5	0

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 A 650



Ligand NAD B 660



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	506/533 (94%)	0.54	52 (10%)	6	6	26, 53, 91, 91	0
1	B	498/533 (93%)	0.77	67 (13%)	3	2	27, 56, 91, 91	0
All	All	1004/1066 (94%)	0.66	119 (11%)	4	4	26, 54, 91, 91	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	467	VAL	9.9
1	B	404	TYR	8.7
1	B	392	LEU	8.3
1	B	402	ILE	7.4
1	B	399	CYS	7.2
1	A	392	LEU	7.1
1	A	405	MET	6.9
1	A	381	ILE	6.9
1	B	469	GLU	6.7
1	A	404	TYR	6.6
1	B	468	LYS	6.6
1	B	400	ILE	6.6
1	A	193	ALA	6.5
1	B	394	LYS	6.4
1	A	194	ASN	6.2
1	B	348	SER	6.2
1	B	393	GLY	6.1
1	A	396	VAL	5.9
1	B	466	PRO	5.8
1	A	400	ILE	5.6
1	A	377	ILE	5.1
1	A	9	ILE	5.1
1	B	380	ILE	5.0
1	B	390	ASP	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	391	LYS	5.0
1	A	378	ASP	4.9
1	B	391	LYS	4.8
1	A	402	ILE	4.8
1	B	382	ALA	4.7
1	B	193	ALA	4.7
1	B	194	ASN	4.6
1	B	396	VAL	4.6
1	B	317	ALA	4.6
1	A	393	GLY	4.6
1	B	389	ASN	4.6
1	A	390	ASP	4.5
1	B	497	PHE	4.4
1	A	406	LYS	4.4
1	B	471	ALA	4.4
1	B	352	LEU	4.4
1	A	398	HIS	4.3
1	B	500	VAL	4.2
1	B	385	ASP	4.1
1	A	385	ASP	4.1
1	A	382	ALA	4.1
1	B	351	HIS	4.0
1	B	470	ASP	4.0
1	B	403	LYS	3.9
1	B	349	TYR	3.9
1	A	380	ILE	3.9
1	B	398	HIS	3.9
1	A	379	ASP	3.8
1	A	192	ALA	3.8
1	B	381	ILE	3.8
1	B	397	ASP	3.8
1	A	376	VAL	3.7
1	A	40	THR	3.7
1	B	408	VAL	3.7
1	A	394	LYS	3.6
1	B	499	PRO	3.6
1	B	386	ILE	3.5
1	B	410	ASP	3.4
1	B	395	LYS	3.4
1	B	197	GLU	3.3
1	A	41	ALA	3.3
1	A	208	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	397	ASP	3.3
1	B	347	ALA	3.3
1	B	405	MET	3.3
1	A	386	ILE	3.2
1	B	40	THR	3.1
1	A	407	PRO	3.1
1	B	21	TYR	3.1
1	A	408	VAL	3.1
1	B	383	SER	3.0
1	A	389	ASN	3.0
1	B	409	GLY	3.0
1	A	399	CYS	3.0
1	B	465	ASP	3.0
1	B	23	ASP	2.9
1	A	395	LYS	2.9
1	B	407	PRO	2.9
1	A	388	TYR	2.8
1	A	195	GLN	2.8
1	B	192	ALA	2.8
1	B	498	HIS	2.8
1	A	355	ASN	2.7
1	B	384	ASN	2.7
1	A	197	GLU	2.6
1	B	350	ASN	2.5
1	B	388	TYR	2.5
1	B	495	PRO	2.5
1	B	208	LYS	2.5
1	B	242	LEU	2.5
1	A	259	ASP	2.4
1	A	15	VAL	2.4
1	B	406	LYS	2.4
1	A	352	LEU	2.4
1	A	533	LEU	2.3
1	A	401	VAL	2.3
1	B	41	ALA	2.3
1	B	533	LEU	2.3
1	B	401	VAL	2.3
1	B	353	GLY	2.3
1	B	45	PHE	2.3
1	B	472	GLY	2.3
1	A	460	SER	2.2
1	A	412	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	474	PHE	2.2
1	A	42	SER	2.2
1	A	351	HIS	2.2
1	A	44	ARG	2.2
1	B	346	ILE	2.1
1	A	497	PHE	2.1
1	A	470	ASP	2.1
1	A	123	GLY	2.1
1	B	488	LEU	2.1
1	B	293	ILE	2.1
1	A	383	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

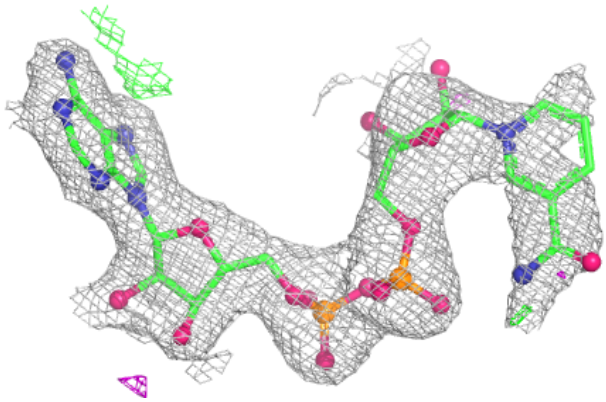
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

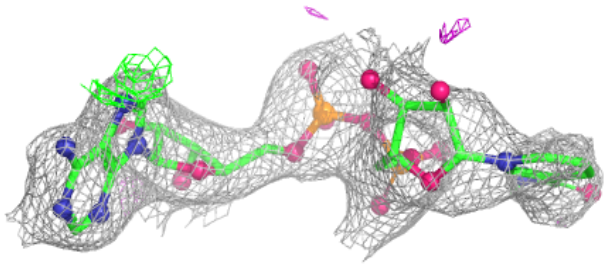
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	A	650	44/44	0.95	0.18	36,57,84,86	0
2	NAD	B	660	44/44	0.95	0.20	43,56,79,81	0

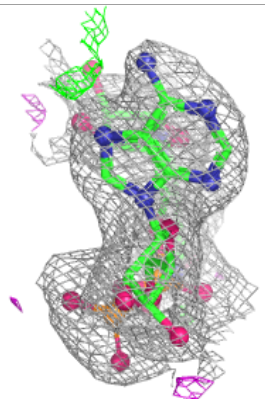
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 650:

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

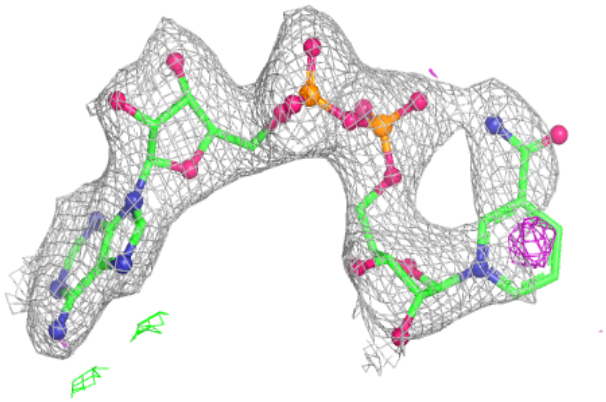


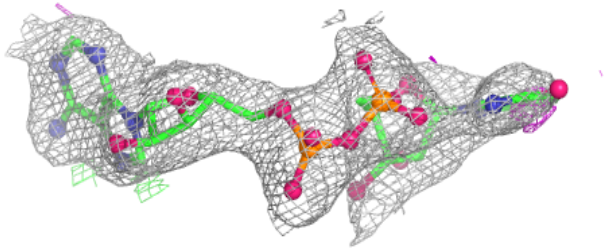


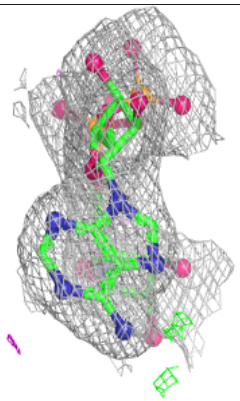


Electron density around NAD B 660:

$2mF_o$-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.