Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:09 pm BST

PDB ID	:	1P1H
Title	:	Crystal structure of the 1L-myo-inositol/NAD+ complex
Authors	:	Jin, X.; Geiger, J.H.
Deposited on	:	2003-04-12
Resolution	:	1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

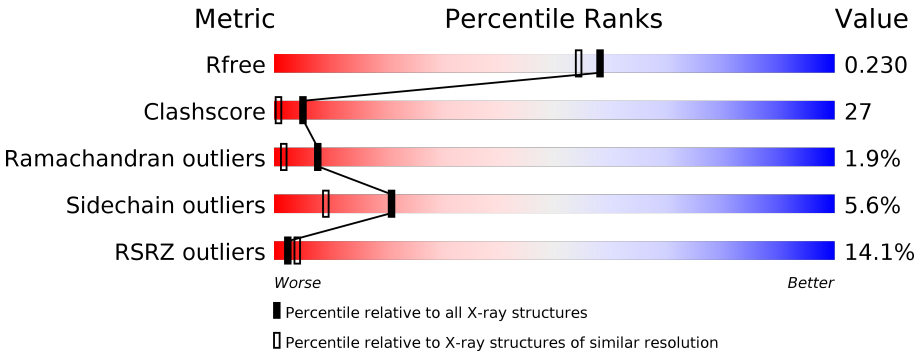
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 on 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	14% 56% 35% 5% 5%
1	B	533	14% 54% 34% • 8%
1	C	533	13% 58% 34% 5% •
1	D	533	12% 52% 34% 5% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17489 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
1	A	506	Total	C	N	O	S	0	0	0
			3988	2538	669	765	16			
1	B	491	Total	C	N	O	S	0	0	0
			3876	2467	652	741	16			
1	C	517	Total	C	N	O	S	0	0	0
			4081	2596	686	783	16			
1	D	487	Total	C	N	O	S	0	0	0
			3839	2439	643	743	14			

There are 40 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
C	?	-	ARG	SEE REMARK 999	UNP P11986

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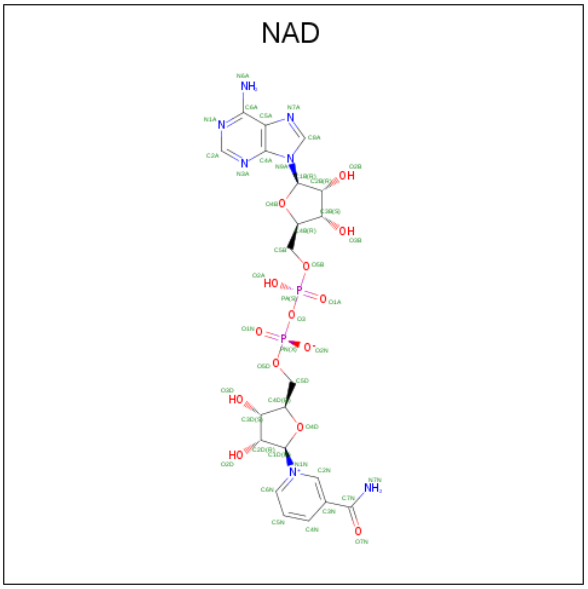
Chain	Residue	Modelled	Actual	Comment	Reference
C	14	VAL	LEU	SEE REMARK 999	UNP P11986
C	?	-	PHE	SEE REMARK 999	UNP P11986
C	60	LEU	GLU	SEE REMARK 999	UNP P11986
C	?	-	ALA	SEE REMARK 999	UNP P11986
C	98	GLU	LYS	SEE REMARK 999	UNP P11986
C	140	ASN	LYS	SEE REMARK 999	UNP P11986
C	141	ASP	HIS	SEE REMARK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

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



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

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

- Molecule 3 is water.

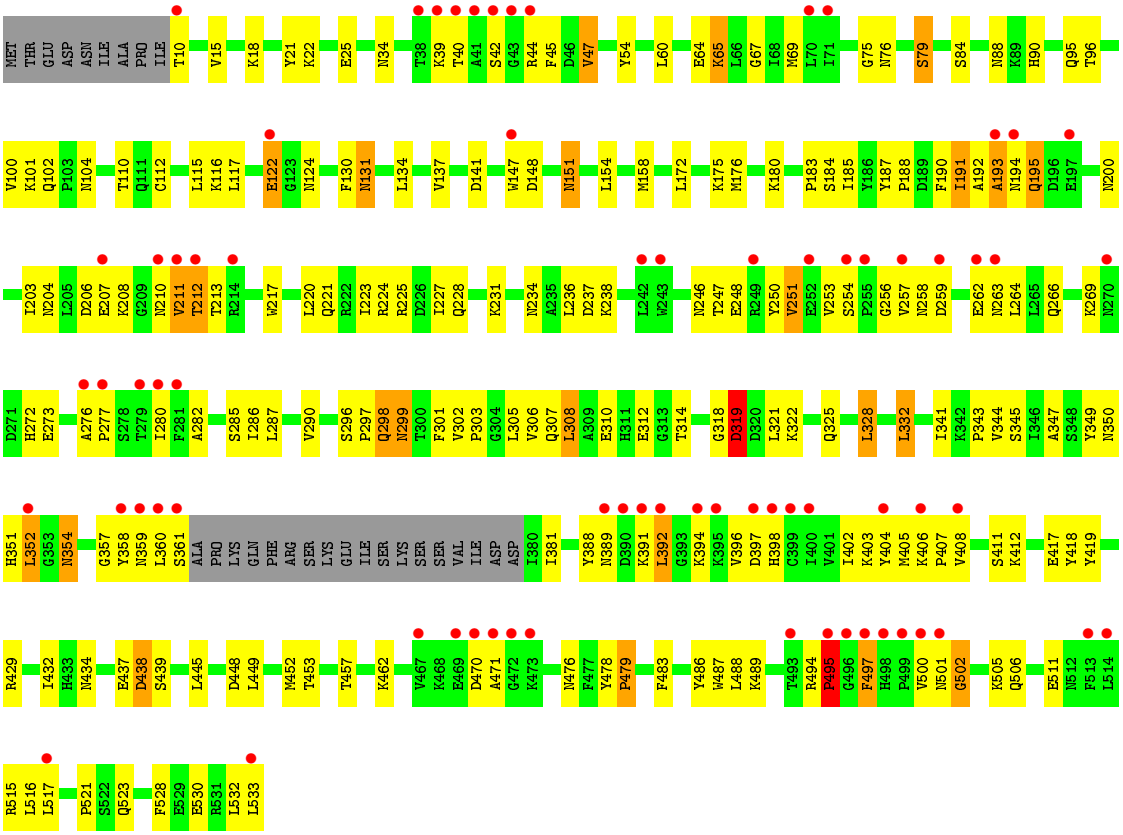
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	425	Total	O	0	0
			425	425		
3	B	354	Total	O	0	0
			354	354		
3	C	383	Total	O	0	0
			383	383		
3	D	367	Total	O	0	0
			367	367		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

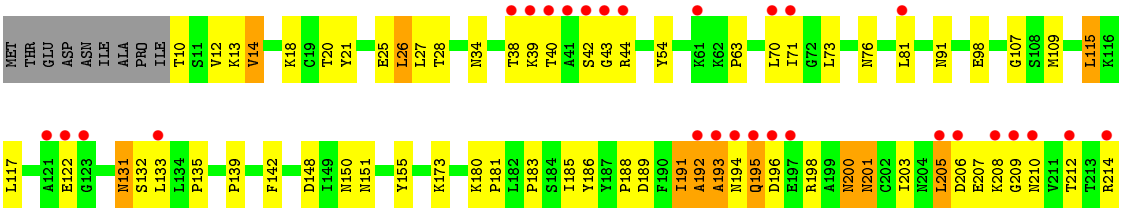
- Molecule 1: Inositol-3-phosphate synthase

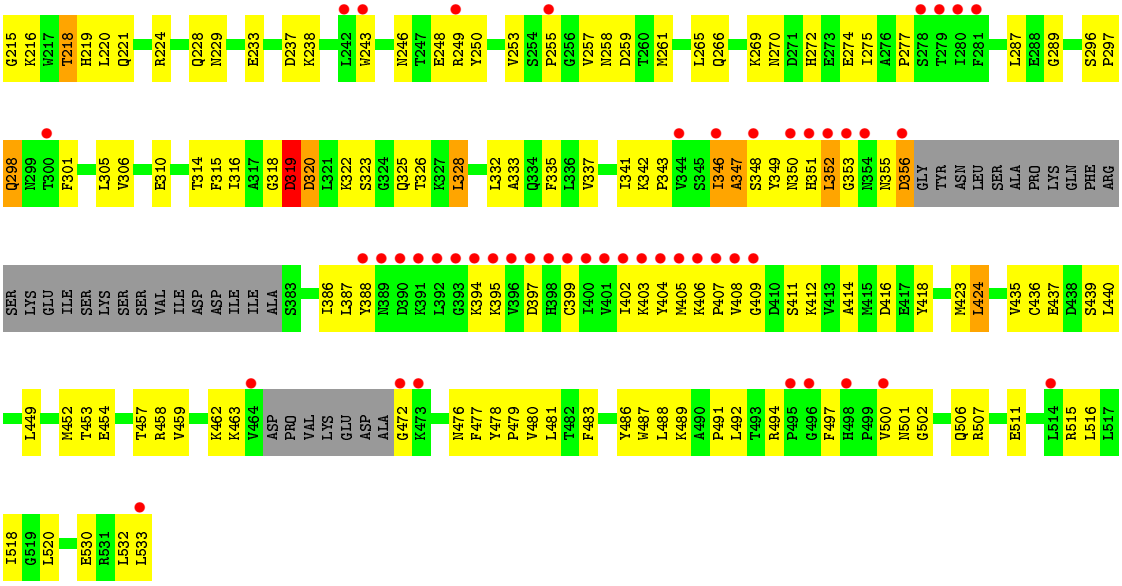
Chain A:



- Molecule 1: Inositol-3-phosphate synthase

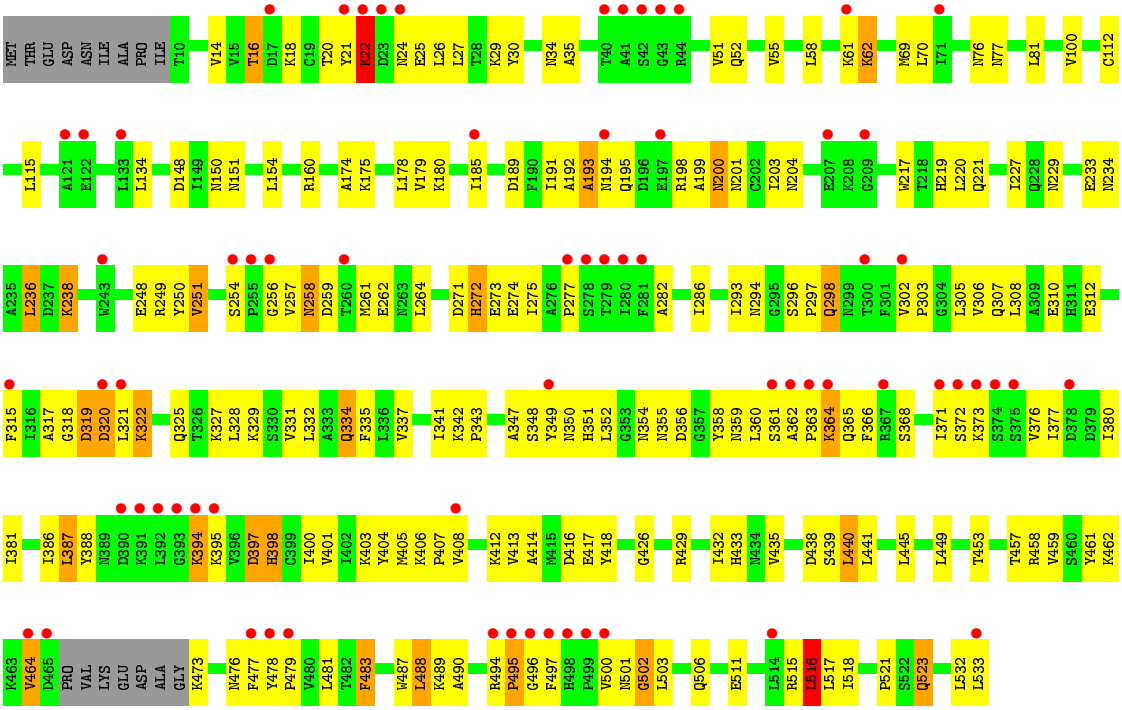
Chain B:





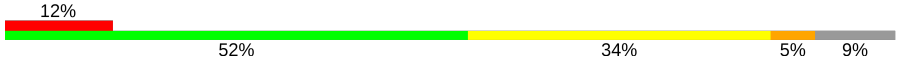
• Molecule 1: Inositol-3-phosphate synthase

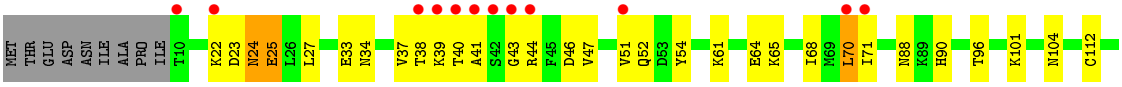
Chain C:

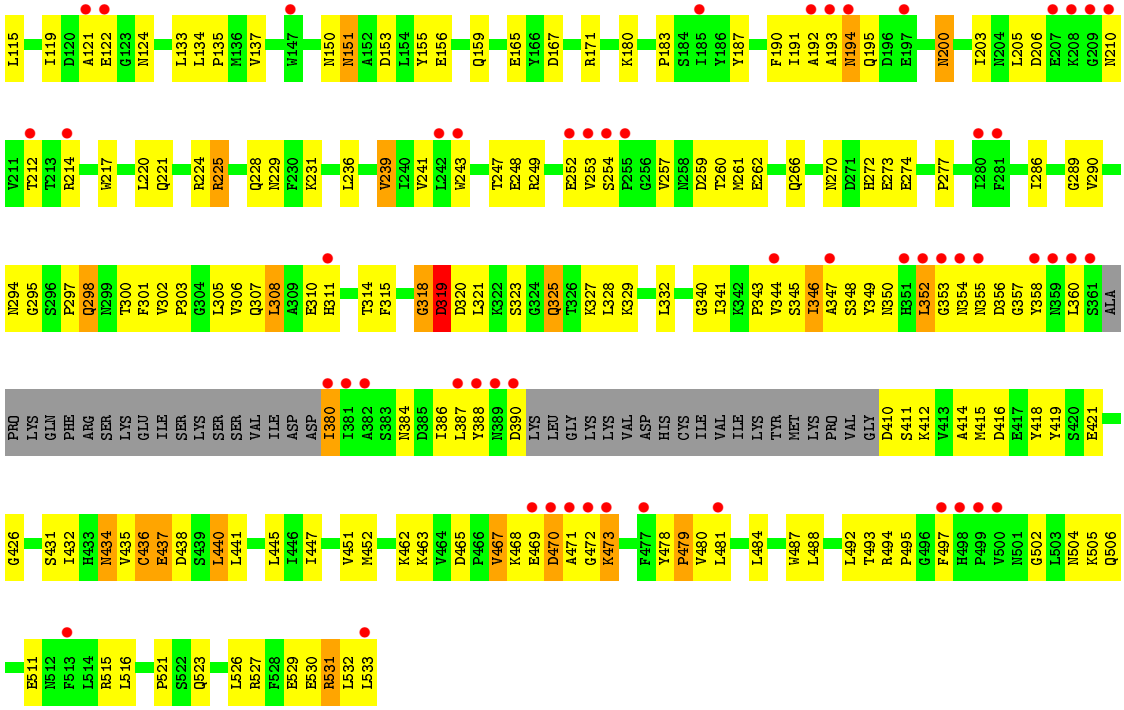


• Molecule 1: Inositol-3-phosphate synthase

Chain D:






L115 I119 D120 A121 E122 G123 N124 L133 L134 P135 M136 V137 W147 N150 N151 A152 D153 L154 Y155 E156 Q159 E165 Y166 D167 R171 K180 P183 S184 I185 Y186 Y187 F190 I191 A192 A193 N194 Q195 D196 E197 N200 I203 N204 L205 D206 E207 K208 G209 N210
V211 T212 T213 R214 W217 L220 Q221 R224 R225 Q228 N229 F230 K231 L236 V239 I240 V241 I242 W243 T247 E248 R249 E252 V253 S254 P255 G256 V257 N258 D259 T260 M261 E262 Q266 N270 D271 H272 E273 E274 P277 I280 F281 I286 G289 V290
N294 G295 S296 P297 Q298 N299 T300 F301 V302 P303 G304 L305 V306 Q307 L308 A309 E310 H311 T314 F315 G318 D319 D320 L321 K322 S323 G324 Q325 T326 K327 L328 K329 L332 G340 I341 K342 P343 V344 S345 I346 A347 S348 Y349 N350 E351 L352 G353 N354 N355 D356 G357 Y358 N359 L360 S361 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 LYS LEU GLY LYS LYS VAL ASP HIS CYS ILE VAL ILE LYS TYR MET LYS PRO VAL GLY D410 S411 K412 V413 A414 M415 D416 E417 Y418 Y419 S420 E421
G426 S431 I432 H433 N434 V435 C436 E437 D438 S439 L440 L441 L445 I446 I447 V451 M452 K462 K463 V464 D465 P466 V467 K468 E469 D470 A471 G472 K473 F477 Y478 P479 V480 L481 L484 W487 L488 L492 T493 R494 P495 G496 F497 H498 P499 V500 N501 G502 L503 N504 K505 Q506
E511 N512 F513 L514 R515 L516 P521 S522 Q523 L526 R527 F528 E529 E530 R531 L532 L533

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.79Å 185.58Å 94.08Å 90.00° 114.77° 90.00°	Depositor
Resolution (Å)	10.00 – 1.95 26.35 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.95) 96.3 (26.35-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.249 0.232 , 0.230	Depositor DCC
R_{free} test set	10775 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 89.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17489	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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

5.1 Standard geometry

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	0.35	0/4066	0.61	0/5513
1	B	0.35	0/3951	0.60	0/5354
1	C	0.36	0/4160	0.60	1/5637 (0.0%)
1	D	0.37	0/3913	0.62	1/5308 (0.0%)
All	All	0.36	0/16090	0.61	2/21812 (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	D	318	GLY	N-CA-C	5.40	126.59	113.10
1	C	516	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3988	0	3989	213	0
1	B	3876	0	3879	220	0
1	C	4081	0	4088	258	0
1	D	3839	0	3816	229	0
2	A	44	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	26	3	0
2	C	44	0	26	5	0
2	D	44	0	26	1	0
3	A	425	0	0	27	0
3	B	354	0	0	20	0
3	C	383	0	0	25	0
3	D	367	0	0	18	0
All	All	17489	0	15876	856	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 27.

All (856) 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:C:494:ARG:HB3	1:C:495:PRO:HD2	1.34	1.08
1:C:494:ARG:HH22	1:D:533:LEU:HB3	0.94	1.06
1:A:352:LEU:HD21	1:A:357:GLY:HA3	1.37	1.06
1:C:69:MET:HE1	1:C:227:ILE:HG12	1.42	1.01
1:D:191:ILE:HG22	1:D:192:ALA:H	1.25	1.01
1:A:69:MET:HE1	1:A:227:ILE:HA	1.42	1.00
1:B:191:ILE:HG13	1:B:192:ALA:H	1.20	1.00
1:C:320:ASP:HB3	1:C:489:LYS:HB3	1.39	1.00
1:C:494:ARG:NH2	1:D:533:LEU:HB3	1.78	0.97
1:B:322:LYS:HA	1:B:489:LYS:HG3	1.46	0.96
1:A:318:GLY:HA2	1:A:488:LEU:HG	1.48	0.96
1:B:437:GLU:HG3	1:B:440:LEU:HD12	1.47	0.94
1:A:115:LEU:HD22	1:A:511:GLU:HG3	1.50	0.93
1:D:437:GLU:HG3	1:D:440:LEU:HD22	1.49	0.93
1:A:502:GLY:HA3	1:A:505:LYS:HE2	1.50	0.93
1:C:533:LEU:HB3	1:D:494:ARG:HH22	1.36	0.90
1:B:323:SER:H	1:B:489:LYS:HE3	1.36	0.89
1:C:494:ARG:HH22	1:D:533:LEU:CB	1.83	0.89
1:B:347:ALA:HA	1:B:399:CYS:HB3	1.53	0.89
1:C:302:VAL:HG22	1:C:303:PRO:HD2	1.57	0.87
1:B:151:ASN:H	1:B:200:ASN:HD21	1.21	0.87
1:D:22:LYS:HE3	1:D:27:LEU:HD11	1.57	0.86
1:C:22:LYS:HZ2	1:C:25:GLU:HB2	1.41	0.85
1:B:289:GLY:HA2	1:B:314:THR:HG21	1.59	0.84
1:B:408:VAL:HG21	3:B:1000:HOH:O	1.76	0.84
1:C:533:LEU:HD13	1:D:494:ARG:HH12	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ILE:HG13	1:B:192:ALA:N	1.92	0.84
1:C:24:ASN:HD22	1:C:61:LYS:HB2	1.42	0.84
1:A:381:ILE:HD11	1:A:396:VAL:HG23	1.58	0.84
1:C:337:VAL:HG21	1:C:380:ILE:HG23	1.57	0.83
1:D:225:ARG:HH21	1:D:229:ASN:HB2	1.42	0.83
1:D:415:MET:HE3	1:D:431:SER:HB2	1.62	0.82
1:B:198:ARG:HD2	3:B:973:HOH:O	1.79	0.82
1:D:40:THR:HG21	1:D:44:ARG:NH1	1.95	0.82
1:C:254:SER:HB2	1:C:257:VAL:HG11	1.62	0.81
1:B:195:GLN:HG3	1:B:198:ARG:HH21	1.43	0.81
1:D:115:LEU:HD22	1:D:511:GLU:HG3	1.60	0.80
1:C:515:ARG:NH1	1:C:521:PRO:O	2.15	0.80
1:D:325:GLN:HA	1:D:325:GLN:HE21	1.45	0.80
1:D:352:LEU:HA	1:D:412:LYS:HA	1.64	0.79
1:C:261:MET:HG2	1:C:307:GLN:NE2	1.97	0.79
1:D:191:ILE:HG22	1:D:192:ALA:N	1.98	0.78
1:C:310:GLU:HG2	1:C:479:PRO:HG2	1.65	0.78
1:C:494:ARG:HB3	1:C:495:PRO:CD	2.13	0.78
1:B:342:LYS:HB2	1:B:387:LEU:HD22	1.66	0.78
1:C:347:ALA:HB2	3:C:920:HOH:O	1.82	0.78
1:C:494:ARG:HH12	1:D:533:LEU:HG	1.49	0.78
1:C:302:VAL:CG2	1:C:303:PRO:HD2	2.14	0.78
1:D:306:VAL:O	1:D:310:GLU:HG3	1.83	0.78
1:A:532:LEU:HB3	1:A:533:LEU:HD12	1.66	0.78
1:C:191:ILE:HG22	1:C:192:ALA:H	1.48	0.77
1:A:389:ASN:HD21	1:A:392:LEU:HD21	1.48	0.77
1:C:191:ILE:HG22	1:C:192:ALA:N	1.99	0.77
1:B:20:THR:HB	1:B:27:LEU:HB2	1.65	0.76
1:C:69:MET:CE	1:C:227:ILE:HG12	2.13	0.76
1:D:352:LEU:HD11	1:D:357:GLY:HA3	1.66	0.76
1:B:212:THR:HG22	1:B:214:ARG:H	1.49	0.76
1:C:151:ASN:H	1:C:200:ASN:HD21	1.30	0.76
1:B:478:TYR:HD2	1:B:480:VAL:HG22	1.51	0.76
1:D:156:GLU:HA	1:D:159:GLN:HE21	1.51	0.76
1:D:318:GLY:HA2	1:D:488:LEU:HD13	1.68	0.76
1:C:478:TYR:HB2	1:C:494:ARG:HH21	1.52	0.74
1:A:251:VAL:H	1:A:299:ASN:HD21	1.35	0.74
1:D:515:ARG:NH1	1:D:521:PRO:O	2.21	0.74
1:A:352:LEU:HD23	1:A:354:ASN:ND2	2.02	0.74
1:C:322:LYS:CD	1:C:327:LYS:HG2	2.18	0.73
1:D:33:GLU:HG2	1:D:51:VAL:HG22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LYS:HB3	1:C:458:ARG:CZ	2.19	0.73
1:B:248:GLU:H	1:B:298:GLN:HG2	1.50	0.73
1:C:500:VAL:HG21	1:D:527:ARG:NE	2.04	0.73
1:C:264:LEU:HD21	1:C:305:LEU:HD13	1.69	0.73
1:C:377:ILE:O	1:C:381:ILE:HG13	1.88	0.72
1:B:310:GLU:HG2	1:B:479:PRO:HG3	1.70	0.72
1:A:407:PRO:HG3	1:C:395:LYS:HE2	1.72	0.72
1:B:205:LEU:HA	1:B:210:ASN:O	1.90	0.72
1:A:352:LEU:CD2	1:A:357:GLY:HA3	2.18	0.72
1:B:478:TYR:CD2	1:B:480:VAL:HG22	2.25	0.71
1:C:533:LEU:HD13	1:D:494:ARG:NH1	2.05	0.71
1:B:437:GLU:HG3	1:B:440:LEU:CD1	2.21	0.71
1:D:352:LEU:HB3	1:D:412:LYS:HB2	1.72	0.71
1:C:320:ASP:CB	1:C:489:LYS:HB3	2.19	0.71
1:B:318:GLY:O	1:B:319:ASP:HB2	1.91	0.70
1:A:221:GLN:HG2	3:A:881:HOH:O	1.90	0.70
1:B:14:VAL:HG11	1:B:518:ILE:O	1.90	0.70
1:C:272:HIS:CD2	1:C:274:GLU:H	2.09	0.70
1:D:310:GLU:HG2	1:D:479:PRO:HG3	1.73	0.70
1:A:352:LEU:HD21	1:A:357:GLY:CA	2.19	0.70
1:C:337:VAL:HG21	1:C:380:ILE:CG2	2.21	0.70
1:A:256:GLY:HA2	1:A:263:ASN:HD22	1.56	0.69
1:C:334:GLN:HG2	1:C:335:PHE:N	2.05	0.69
1:C:373:LYS:HE3	1:C:489:LYS:HD3	1.72	0.69
1:D:532:LEU:O	1:D:533:LEU:HB2	1.90	0.69
1:D:415:MET:CE	1:D:431:SER:HB2	2.23	0.69
1:C:150:ASN:ND2	1:C:160:ARG:HH12	1.90	0.69
1:C:331:VAL:HA	1:C:334:GLN:NE2	2.06	0.69
1:A:257:VAL:HG13	1:A:258:ASN:H	1.58	0.69
1:C:115:LEU:CD2	1:C:511:GLU:HG2	2.23	0.69
1:A:328:LEU:HD13	3:A:935:HOH:O	1.92	0.68
1:A:39:LYS:O	1:A:40:THR:HG23	1.93	0.68
1:A:486:TYR:HA	1:A:506:GLN:NE2	2.09	0.68
1:B:318:GLY:HA2	1:B:488:LEU:HD13	1.76	0.68
1:A:64:GLU:O	1:A:65:LYS:HD2	1.93	0.67
1:C:22:LYS:HB3	1:C:22:LYS:HZ2	1.59	0.67
1:A:254:SER:O	1:A:257:VAL:HG12	1.94	0.67
1:C:154:LEU:HD22	1:C:179:VAL:HG11	1.77	0.67
1:C:350:ASN:HD22	1:C:412:LYS:HE3	1.59	0.67
1:A:318:GLY:O	1:A:319:ASP:HB2	1.93	0.67
1:C:515:ARG:HD2	3:C:911:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ALA:HB3	1:C:365:GLN:HG2	1.77	0.67
1:A:10:THR:HG22	1:B:43:GLY:HA3	1.76	0.67
1:C:154:LEU:HD22	1:C:179:VAL:CG1	2.25	0.67
1:C:494:ARG:CB	1:C:495:PRO:HD2	2.20	0.67
1:B:404:TYR:OH	1:B:406:LYS:HE3	1.94	0.66
1:C:70:LEU:HD11	1:C:81:LEU:HD23	1.76	0.66
1:A:217:TRP:O	1:A:221:GLN:HG3	1.95	0.66
1:C:478:TYR:CD1	1:C:479:PRO:HD2	2.31	0.66
1:C:533:LEU:HB3	1:D:494:ARG:NH2	2.08	0.66
1:B:352:LEU:H	1:B:352:LEU:HD13	1.61	0.66
1:B:98:GLU:HB2	3:B:806:HOH:O	1.95	0.66
1:C:296:SER:HB2	1:C:298:GLN:OE1	1.96	0.66
1:D:437:GLU:HG3	1:D:440:LEU:CD2	2.24	0.66
1:B:388:TYR:HB3	1:B:394:LYS:HA	1.77	0.66
1:D:38:THR:HG23	1:D:46:ASP:HB2	1.76	0.66
1:A:256:GLY:HA2	1:A:263:ASN:ND2	2.10	0.65
1:D:191:ILE:CG2	1:D:192:ALA:H	2.06	0.65
1:D:341:ILE:O	1:D:343:PRO:HD3	1.95	0.65
1:A:151:ASN:HB2	1:A:180:LYS:HE2	1.77	0.65
1:C:115:LEU:HD21	1:C:511:GLU:HG2	1.78	0.65
1:D:318:GLY:CA	1:D:488:LEU:HD13	2.26	0.65
1:B:405:MET:SD	1:D:347:ALA:HB2	2.36	0.65
1:C:321:LEU:O	1:C:321:LEU:HD23	1.96	0.65
1:A:47:VAL:HG22	1:B:14:VAL:HA	1.79	0.65
1:D:273:GLU:HG2	3:D:822:HOH:O	1.96	0.65
1:D:434:ASN:HD22	1:D:435:VAL:N	1.95	0.65
1:C:178:LEU:HD12	3:C:936:HOH:O	1.95	0.65
1:C:322:LYS:HA	1:C:489:LYS:HE3	1.79	0.64
1:D:318:GLY:O	1:D:319:ASP:HB2	1.96	0.64
1:A:322:LYS:NZ	1:A:506:GLN:HE22	1.95	0.64
1:D:345:SER:HB3	1:D:419:TYR:HB3	1.78	0.64
1:D:473:LYS:HA	3:D:895:HOH:O	1.97	0.64
1:B:322:LYS:NZ	1:B:506:GLN:HE22	1.96	0.64
1:B:486:TYR:HA	1:B:506:GLN:NE2	2.13	0.64
1:C:361:SER:HB2	3:C:1031:HOH:O	1.97	0.63
1:C:191:ILE:HG21	1:C:195:GLN:HG3	1.80	0.63
1:A:505:LYS:HG3	3:A:777:HOH:O	1.97	0.63
1:C:322:LYS:HD3	1:C:327:LYS:HG2	1.79	0.63
1:B:195:GLN:HG3	1:B:198:ARG:NH2	2.14	0.63
1:C:14:VAL:HG22	1:D:47:VAL:HB	1.79	0.63
1:B:409:GLY:HA3	3:B:844:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:GLY:HA3	1:D:440:LEU:HD23	1.81	0.63
1:C:322:LYS:HA	1:C:489:LYS:HB2	1.80	0.63
1:B:405:MET:O	1:B:408:VAL:HG22	1.99	0.62
1:B:353:GLY:HA3	1:B:406:LYS:HA	1.80	0.62
1:B:395:LYS:HE2	1:B:397:ASP:OD2	1.99	0.62
1:C:302:VAL:HG22	1:C:303:PRO:CD	2.29	0.62
1:A:405:MET:HE2	3:C:920:HOH:O	1.99	0.62
1:C:248:GLU:OE1	1:C:277:PRO:HD2	2.00	0.62
1:D:321:LEU:HB3	3:D:712:HOH:O	2.00	0.62
1:A:321:LEU:HD22	1:A:445:LEU:CD2	2.30	0.62
1:A:478:TYR:CD2	1:A:479:PRO:HD2	2.34	0.62
1:B:395:LYS:HD2	3:B:825:HOH:O	1.99	0.62
1:C:151:ASN:N	1:C:200:ASN:HD21	1.97	0.62
1:C:248:GLU:H	1:C:298:GLN:HG2	1.65	0.62
1:C:445:LEU:HD21	1:C:487:TRP:HB3	1.82	0.62
1:B:12:VAL:HG21	1:B:133:LEU:HD23	1.83	0.61
1:D:329:LYS:HD2	1:D:416:ASP:OD2	2.00	0.61
1:C:58:LEU:HD22	1:C:134:LEU:HD13	1.80	0.61
1:D:357:GLY:O	1:D:360:LEU:HB3	2.00	0.61
1:B:341:ILE:O	1:B:343:PRO:HD3	2.00	0.61
1:C:328:LEU:O	1:C:332:LEU:HG	2.01	0.61
1:B:186:TYR:OH	1:B:196:ASP:HA	2.01	0.61
1:B:191:ILE:CG1	1:B:192:ALA:H	2.02	0.61
1:A:392:LEU:HB3	3:B:854:HOH:O	2.00	0.61
1:B:195:GLN:H	1:B:195:GLN:NE2	1.98	0.61
1:D:192:ALA:HA	3:D:970:HOH:O	2.00	0.61
1:B:109:MET:HE2	1:B:507:ARG:HE	1.65	0.60
1:B:478:TYR:CD1	1:B:479:PRO:HD2	2.36	0.60
1:D:289:GLY:HA2	1:D:314:THR:CG2	2.31	0.60
1:A:501:ASN:HA	1:A:506:GLN:OE1	2.01	0.60
1:C:387:LEU:HD11	1:D:112:CYS:HB3	1.82	0.60
1:A:332:LEU:HD21	1:B:328:LEU:HD12	1.82	0.60
1:C:432:ILE:HG13	3:C:1034:HOH:O	2.01	0.60
1:B:480:VAL:O	1:B:480:VAL:HG23	2.01	0.60
1:D:225:ARG:NH2	1:D:229:ASN:HB2	2.14	0.60
1:D:289:GLY:HA2	1:D:314:THR:HG21	1.83	0.60
1:C:394:LYS:NZ	1:C:394:LYS:HB3	2.17	0.60
1:C:478:TYR:CB	1:C:494:ARG:HH21	2.14	0.60
1:A:257:VAL:HG13	1:A:258:ASN:N	2.15	0.60
1:A:449:LEU:HD21	1:A:487:TRP:HB2	1.82	0.60
1:B:325:GLN:HA	1:B:325:GLN:HE21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:VAL:HG12	3:C:797:HOH:O	2.00	0.60
1:D:96:THR:HG22	1:D:165:GLU:HG2	1.84	0.60
1:A:341:ILE:O	1:A:343:PRO:HD3	2.01	0.60
1:B:70:LEU:HD11	1:B:81:LEU:HD23	1.84	0.60
1:A:75:GLY:O	1:A:79:SER:HB2	2.01	0.60
1:C:22:LYS:NZ	1:C:25:GLU:HB2	2.16	0.60
1:D:511:GLU:O	1:D:515:ARG:HG3	2.02	0.60
1:C:150:ASN:HA	1:C:200:ASN:ND2	2.17	0.59
1:B:437:GLU:CG	1:B:440:LEU:HD12	2.28	0.59
1:C:453:THR:O	1:C:457:THR:HG23	2.02	0.59
1:A:352:LEU:N	1:A:352:LEU:HD13	2.17	0.59
1:D:412:LYS:HE3	1:D:438:ASP:OD1	2.02	0.59
1:A:286:ILE:HG22	1:A:312:GLU:HG3	1.84	0.59
1:B:200:ASN:C	1:B:200:ASN:HD22	2.05	0.59
1:B:266:GLN:HE21	1:B:270:ASN:HD21	1.48	0.59
1:C:440:LEU:HD23	1:D:426:GLY:HA3	1.84	0.59
1:C:325:GLN:NE2	1:C:412:LYS:HD3	2.17	0.59
1:C:329:LYS:HG3	1:C:418:TYR:OH	2.03	0.59
1:D:344:VAL:HG11	1:D:421:GLU:OE2	2.03	0.59
1:B:42:SER:C	1:B:44:ARG:H	2.06	0.59
1:C:273:GLU:H	1:C:273:GLU:CD	2.05	0.59
1:B:215:GLY:O	1:B:218:THR:HB	2.02	0.59
1:A:116:LYS:HB3	1:A:523:GLN:NE2	2.18	0.59
1:A:310:GLU:HG2	1:A:479:PRO:HG3	1.84	0.59
1:C:18:LYS:HE2	3:C:820:HOH:O	2.03	0.59
1:B:185:ILE:HG12	1:B:203:ILE:HD11	1.85	0.59
1:C:258:ASN:HD22	1:C:258:ASN:C	2.07	0.59
1:C:325:GLN:HB3	3:C:1035:HOH:O	2.02	0.59
1:A:332:LEU:HG	1:A:432:ILE:HD11	1.84	0.58
1:A:21:TYR:HD2	1:A:60:LEU:HD11	1.67	0.58
1:A:438:ASP:HB3	2:A:650:NAD:O7N	2.03	0.58
1:C:516:LEU:HD23	1:C:516:LEU:C	2.22	0.58
1:A:220:LEU:HD23	1:A:280:ILE:HG23	1.85	0.58
1:C:191:ILE:CG2	1:C:195:GLN:HG3	2.33	0.58
1:C:523:GLN:HA	1:C:523:GLN:HE21	1.67	0.58
1:B:193:ALA:N	1:B:196:ASP:HB2	2.17	0.58
1:C:254:SER:HB2	1:C:257:VAL:CG1	2.32	0.58
1:A:405:MET:HE3	1:C:397:ASP:HB3	1.84	0.58
1:B:318:GLY:CA	1:B:488:LEU:HD13	2.33	0.58
1:C:272:HIS:HB3	1:C:275:ILE:HG12	1.85	0.58
1:C:319:ASP:HB3	1:C:490:ALA:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:SER:H	1:B:489:LYS:CE	2.12	0.58
1:A:351:HIS:HD2	1:C:349:TYR:OH	1.87	0.58
1:C:351:HIS:HA	1:C:403:LYS:O	2.03	0.58
1:A:264:LEU:HD21	1:A:305:LEU:HD13	1.86	0.58
1:B:63:PRO:HG3	1:B:238:LYS:HG3	1.85	0.58
1:C:302:VAL:O	1:C:306:VAL:HG23	2.04	0.58
1:C:494:ARG:HH12	1:D:533:LEU:CG	2.16	0.58
1:D:346:ILE:HG12	1:D:418:TYR:CD2	2.38	0.58
1:A:47:VAL:HG22	1:B:14:VAL:HB	1.85	0.57
1:D:411:SER:HB3	3:D:867:HOH:O	2.04	0.57
1:B:478:TYR:CE2	1:B:494:ARG:HG2	2.38	0.57
1:C:191:ILE:CG2	1:C:192:ALA:H	2.16	0.57
1:B:306:VAL:O	1:B:310:GLU:HG3	2.04	0.57
1:D:286:ILE:HG21	1:D:308:LEU:HD13	1.84	0.57
1:C:25:GLU:HB3	3:C:922:HOH:O	2.03	0.57
1:C:192:ALA:O	1:C:193:ALA:HB2	2.04	0.57
1:D:122:GLU:HB2	1:D:124:ASN:OD1	2.04	0.57
1:D:325:GLN:HA	1:D:325:GLN:NE2	2.16	0.57
1:A:15:VAL:HG11	3:A:788:HOH:O	2.04	0.57
1:C:302:VAL:HG12	1:C:305:LEU:HB2	1.86	0.57
1:C:297:PRO:HB3	1:C:320:ASP:OD1	2.04	0.57
1:A:497:PHE:CD2	1:B:530:GLU:HG2	2.40	0.56
1:A:462:LYS:HA	3:A:1072:HOH:O	2.05	0.56
1:A:407:PRO:CG	1:C:395:LYS:HE2	2.36	0.56
1:C:405:MET:O	1:C:408:VAL:HG22	2.06	0.56
1:C:221:GLN:HG2	3:C:799:HOH:O	2.06	0.56
1:C:533:LEU:CD1	1:D:494:ARG:HH12	2.14	0.56
1:D:380:ILE:N	1:D:380:ILE:HD13	2.21	0.56
1:C:432:ILE:HD12	1:D:432:ILE:HD12	1.88	0.56
1:A:231:LYS:HE3	3:A:790:HOH:O	2.05	0.56
1:C:350:ASN:ND2	1:C:412:LYS:HE3	2.20	0.56
1:D:183:PRO:HB2	1:D:203:ILE:HG23	1.88	0.56
1:D:38:THR:CG2	1:D:46:ASP:HB2	2.36	0.56
1:D:259:ASP:HA	1:D:303:PRO:HG2	1.88	0.56
1:C:191:ILE:CG2	1:C:192:ALA:N	2.69	0.56
1:A:39:LYS:HB2	1:A:45:PHE:CD1	2.41	0.55
1:B:348:SER:HB3	1:B:399:CYS:O	2.06	0.55
1:C:77:ASN:ND2	2:C:670:NAD:N7N	2.54	0.55
1:B:10:THR:HG22	1:B:132:SER:HB2	1.87	0.55
1:A:124:ASN:HB3	3:B:991:HOH:O	2.05	0.55
1:A:248:GLU:H	1:A:298:GLN:NE2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:LEU:HD23	1:D:220:LEU:C	2.27	0.55
1:D:300:THR:O	1:D:305:LEU:HD12	2.07	0.55
1:D:350:ASN:OD1	1:D:412:LYS:HD3	2.06	0.55
1:B:506:GLN:HG3	3:B:916:HOH:O	2.07	0.55
1:C:417:GLU:OE1	1:C:429:ARG:HD3	2.05	0.55
1:A:256:GLY:CA	1:A:263:ASN:HD22	2.18	0.55
1:D:318:GLY:HA2	1:D:488:LEU:CD1	2.36	0.55
1:B:348:SER:HB2	1:B:416:ASP:OD2	2.07	0.55
1:D:470:ASP:O	1:D:471:ALA:HB3	2.06	0.55
1:B:353:GLY:CA	1:B:406:LYS:HA	2.37	0.55
1:D:321:LEU:HG	1:D:445:LEU:HD22	1.88	0.55
1:A:185:ILE:CD1	1:A:223:ILE:HD11	2.37	0.55
1:A:325:GLN:NE2	3:A:935:HOH:O	2.40	0.55
1:D:478:TYR:CD2	1:D:479:PRO:HD2	2.42	0.55
1:C:403:LYS:NZ	1:C:403:LYS:HB3	2.21	0.55
1:D:191:ILE:HG21	1:D:195:GLN:HG3	1.88	0.55
1:A:351:HIS:HA	1:A:403:LYS:O	2.07	0.54
1:B:155:TYR:CE2	1:B:173:LYS:HE3	2.42	0.54
1:D:40:THR:CG2	1:D:44:ARG:HB3	2.37	0.54
1:C:318:GLY:O	1:C:319:ASP:HB2	2.07	0.54
1:B:76:ASN:HB3	1:B:439:SER:OG	2.07	0.54
1:A:325:GLN:HE22	1:A:434:ASN:HB2	1.72	0.54
1:B:131:ASN:HD22	1:B:131:ASN:C	2.10	0.54
1:B:459:VAL:HB	1:B:477:PHE:HE1	1.73	0.54
1:C:24:ASN:ND2	1:C:61:LYS:HB2	2.19	0.54
1:A:301:PHE:HB2	3:A:942:HOH:O	2.08	0.54
1:C:296:SER:HB3	1:C:297:PRO:HD2	1.89	0.54
1:A:299:ASN:ND2	1:A:299:ASN:H	2.06	0.54
1:A:381:ILE:HD11	1:A:396:VAL:CG2	2.35	0.54
1:D:302:VAL:HB	1:D:303:PRO:HD2	1.88	0.54
1:A:116:LYS:HB3	1:A:523:GLN:HE22	1.72	0.54
1:A:158:MET:CE	1:A:176:MET:HG3	2.37	0.54
1:C:238:LYS:HG2	3:C:1015:HOH:O	2.08	0.54
1:C:354:ASN:HB2	3:C:688:HOH:O	2.08	0.54
1:A:246:ASN:HD22	1:A:359:ASN:ND2	2.06	0.53
1:A:47:VAL:CG2	1:B:14:VAL:HB	2.38	0.53
1:C:341:ILE:O	1:C:343:PRO:HD3	2.08	0.53
1:A:210:ASN:O	1:A:211:VAL:O	2.26	0.53
1:B:117:LEU:HD21	1:B:133:LEU:HD21	1.90	0.53
1:B:20:THR:HG22	1:B:21:TYR:N	2.23	0.53
1:B:352:LEU:HD13	1:B:352:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:GLU:OE2	1:B:458:ARG:HD3	2.08	0.53
1:C:21:TYR:CE2	1:C:26:LEU:HD13	2.43	0.53
1:D:151:ASN:H	1:D:200:ASN:HD21	1.55	0.53
1:D:480:VAL:HG11	1:D:492:LEU:HD22	1.90	0.53
1:C:18:LYS:HA	1:C:29:LYS:HE2	1.90	0.53
1:C:234:ASN:HB2	1:C:236:LEU:HD22	1.90	0.53
1:D:502:GLY:O	1:D:506:GLN:HG3	2.08	0.53
1:D:225:ARG:NH2	3:D:819:HOH:O	2.40	0.53
1:B:325:GLN:HG2	1:B:414:ALA:HB1	1.90	0.53
1:C:352:LEU:H	1:C:352:LEU:HD23	1.74	0.53
1:C:381:ILE:HG23	1:C:388:TYR:CG	2.44	0.53
1:B:224:ARG:O	1:B:228:GLN:HG3	2.09	0.53
1:B:351:HIS:HB3	1:B:403:LYS:HB2	1.91	0.53
1:C:250:TYR:HD1	1:C:368:SER:HG	1.55	0.53
1:D:165:GLU:HG3	3:D:734:HOH:O	2.09	0.53
1:C:58:LEU:HD13	1:C:459:VAL:HG22	1.91	0.53
1:B:346:ILE:HG23	1:B:418:TYR:CE2	2.44	0.53
1:C:325:GLN:HE21	1:C:412:LYS:HD3	1.74	0.53
1:D:206:ASP:HB3	1:D:212:THR:HB	1.90	0.53
1:A:500:VAL:HG22	3:A:943:HOH:O	2.07	0.53
1:B:180:LYS:HE3	3:B:982:HOH:O	2.08	0.53
1:C:533:LEU:HD22	1:D:494:ARG:HH12	1.72	0.53
1:D:224:ARG:O	1:D:228:GLN:HG3	2.09	0.53
1:A:183:PRO:HB2	1:A:203:ILE:HG23	1.91	0.52
1:B:491:PRO:HD2	1:B:501:ASN:HD21	1.74	0.52
1:A:470:ASP:O	1:A:471:ALA:HB3	2.09	0.52
1:B:255:PRO:HA	1:B:259:ASP:OD1	2.09	0.52
1:C:134:LEU:HD21	1:C:518:ILE:HG22	1.91	0.52
1:B:188:PRO:O	1:B:192:ALA:HB2	2.09	0.52
1:B:350:ASN:ND2	1:B:402:ILE:HG12	2.24	0.52
1:C:112:CYS:HB3	1:D:387:LEU:CD1	2.39	0.52
1:C:192:ALA:HB2	1:C:359:ASN:OD1	2.09	0.52
1:C:328:LEU:CD2	1:C:432:ILE:HG21	2.38	0.52
1:D:183:PRO:HB2	1:D:203:ILE:CG2	2.40	0.52
1:D:467:VAL:O	1:D:467:VAL:HG13	2.08	0.52
1:C:532:LEU:HD23	1:D:54:TYR:CE2	2.44	0.52
1:A:67:GLY:HA3	1:A:236:LEU:HD13	1.91	0.52
1:A:360:LEU:HD23	3:A:1059:HOH:O	2.09	0.52
1:B:208:LYS:HE3	3:B:974:HOH:O	2.10	0.52
1:D:360:LEU:O	1:D:360:LEU:HD22	2.10	0.52
1:D:434:ASN:HD22	1:D:434:ASN:C	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:LEU:HD12	1:D:516:LEU:C	2.29	0.52
1:A:272:HIS:ND1	1:A:273:GLU:N	2.57	0.52
1:A:328:LEU:HD21	1:B:332:LEU:CD2	2.39	0.52
1:B:326:THR:OG1	1:B:489:LYS:HE2	2.09	0.52
1:C:294:ASN:HB3	1:C:318:GLY:HA3	1.92	0.52
1:C:400:ILE:HG23	1:C:400:ILE:O	2.10	0.52
1:C:55:VAL:HG23	1:C:464:VAL:HG11	1.90	0.52
1:B:12:VAL:HG21	1:B:133:LEU:CD2	2.40	0.52
1:A:238:LYS:HG3	3:A:1034:HOH:O	2.09	0.52
1:C:373:LYS:CE	1:C:489:LYS:HD3	2.37	0.52
1:D:484:LEU:HA	1:D:487:TRP:CZ3	2.45	0.52
1:A:307:GLN:HA	1:A:310:GLU:OE1	2.09	0.52
1:D:88:ASN:HD21	1:D:104:ASN:CA	2.23	0.52
1:A:206:ASP:HB3	1:A:212:THR:OG1	2.09	0.51
1:A:515:ARG:NH1	1:A:521:PRO:O	2.43	0.51
1:A:417:GLU:OE2	1:A:429:ARG:HD3	2.10	0.51
1:A:341:ILE:HD13	1:B:107:GLY:HA2	1.92	0.51
1:A:502:GLY:HA3	1:A:505:LYS:CE	2.30	0.51
1:C:306:VAL:O	1:C:310:GLU:HG3	2.10	0.51
1:C:348:SER:HA	1:C:416:ASP:OD1	2.11	0.51
1:C:440:LEU:CD2	1:D:426:GLY:HA3	2.40	0.51
1:C:329:LYS:HE2	1:C:348:SER:OG	2.10	0.51
1:D:360:LEU:C	1:D:360:LEU:HD13	2.30	0.51
1:A:358:TYR:O	1:A:361:SER:HB3	2.10	0.51
1:B:301:PHE:CD1	1:B:492:LEU:HD22	2.45	0.51
1:B:301:PHE:HD1	1:B:492:LEU:HD22	1.75	0.51
1:C:478:TYR:HB2	1:C:494:ARG:NH2	2.23	0.51
1:A:405:MET:HG3	3:C:920:HOH:O	2.10	0.51
1:B:325:GLN:NE2	1:B:325:GLN:HA	2.26	0.51
1:C:438:ASP:HB3	2:C:670:NAD:O7N	2.10	0.51
1:D:295:GLY:HA3	1:D:321:LEU:HD13	1.93	0.51
1:D:438:ASP:N	1:D:438:ASP:OD2	2.44	0.51
1:C:347:ALA:HB1	1:C:349:TYR:CE2	2.45	0.51
1:B:248:GLU:OE1	1:B:277:PRO:HD2	2.11	0.51
1:A:350:ASN:HD21	1:A:402:ILE:HG23	1.76	0.50
1:A:437:GLU:HG3	3:A:658:HOH:O	2.11	0.50
1:A:39:LYS:HD2	1:A:45:PHE:CZ	2.46	0.50
1:C:445:LEU:HG	1:C:487:TRP:HD1	1.76	0.50
1:A:306:VAL:O	1:A:310:GLU:HG3	2.11	0.50
1:B:356:ASP:HB2	2:B:660:NAD:H3D	1.93	0.50
1:C:185:ILE:HG12	1:C:203:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:VAL:HG22	1:A:419:TYR:O	2.12	0.50
1:C:282:ALA:HB3	1:C:305:LEU:HD21	1.93	0.50
2:C:670:NAD:O5D	2:C:670:NAD:H2N	2.11	0.50
1:A:296:SER:HA	2:A:650:NAD:O2D	2.11	0.50
1:A:302:VAL:HB	1:A:303:PRO:HD2	1.92	0.50
1:D:340:GLY:O	1:D:387:LEU:HD21	2.10	0.50
1:A:253:VAL:HG13	1:A:253:VAL:O	2.10	0.50
1:B:122:GLU:N	1:B:122:GLU:OE2	2.42	0.50
1:B:150:ASN:HD22	1:B:198:ARG:HG3	1.77	0.50
1:B:310:GLU:HG2	1:B:479:PRO:CG	2.41	0.50
1:A:18:LYS:HE3	3:A:988:HOH:O	2.11	0.50
1:B:476:ASN:HB3	3:B:827:HOH:O	2.10	0.50
1:C:150:ASN:HA	1:C:200:ASN:HD21	1.77	0.50
1:C:354:ASN:OD1	1:C:356:ASP:HB3	2.12	0.50
1:C:433:HIS:HB3	1:D:431:SER:OG	2.12	0.50
1:C:500:VAL:HG11	3:D:864:HOH:O	2.11	0.50
1:C:372:SER:CB	1:C:490:ALA:HB2	2.42	0.50
1:A:286:ILE:HG23	1:A:314:THR:HG21	1.94	0.49
1:B:200:ASN:ND2	1:B:200:ASN:C	2.65	0.49
1:C:319:ASP:O	1:C:320:ASP:HB2	2.11	0.49
1:B:221:GLN:HG2	3:B:983:HOH:O	2.12	0.49
1:C:516:LEU:HD23	1:C:517:LEU:N	2.27	0.49
1:C:51:VAL:HG22	1:C:52:GLN:N	2.27	0.49
1:A:47:VAL:HG22	1:B:14:VAL:CB	2.42	0.49
1:D:40:THR:HG22	1:D:44:ARG:HB3	1.93	0.49
1:A:191:ILE:HD12	1:A:195:GLN:HG2	1.94	0.49
1:D:115:LEU:HD22	1:D:511:GLU:CG	2.39	0.49
1:D:231:LYS:HE2	1:D:239:VAL:HG13	1.94	0.49
3:C:996:HOH:O	1:D:463:LYS:HD2	2.13	0.49
1:A:349:TYR:O	1:A:350:ASN:HB3	2.13	0.49
1:B:216:LYS:HA	1:B:219:HIS:ND1	2.28	0.49
1:B:253:VAL:O	1:B:253:VAL:HG13	2.12	0.49
1:B:272:HIS:HE1	1:B:274:GLU:HG2	1.77	0.49
1:C:180:LYS:HB3	3:C:881:HOH:O	2.11	0.49
1:C:55:VAL:HG23	1:C:464:VAL:CG1	2.42	0.49
1:A:88:ASN:HD21	1:A:104:ASN:CA	2.25	0.49
1:B:491:PRO:CD	1:B:501:ASN:HD21	2.25	0.49
1:C:297:PRO:HB3	1:C:320:ASP:CG	2.33	0.49
1:A:204:ASN:O	1:A:211:VAL:O	2.30	0.49
1:A:408:VAL:HG12	1:A:411:SER:O	2.12	0.49
1:B:272:HIS:CE1	1:B:274:GLU:HG2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:502:GLY:O	1:C:506:GLN:HG3	2.13	0.49
1:D:44:ARG:HB3	1:D:44:ARG:NH1	2.28	0.49
1:A:151:ASN:CB	1:A:180:LYS:HE2	2.42	0.49
1:B:63:PRO:CG	1:B:238:LYS:HG3	2.43	0.49
1:A:211:VAL:O	1:A:212:THR:HB	2.13	0.48
1:A:391:LYS:HD3	3:A:761:HOH:O	2.12	0.48
1:B:296:SER:O	1:B:320:ASP:N	2.46	0.48
1:C:310:GLU:CG	1:C:479:PRO:HG2	2.41	0.48
1:D:68:ILE:HG22	1:D:70:LEU:HD13	1.95	0.48
1:A:88:ASN:HD21	1:A:104:ASN:HA	1.77	0.48
1:B:405:MET:HE3	3:D:874:HOH:O	2.12	0.48
1:B:318:GLY:HA2	1:B:488:LEU:CD1	2.42	0.48
1:C:500:VAL:HG21	1:D:527:ARG:CZ	2.43	0.48
1:D:286:ILE:CG2	1:D:308:LEU:HD13	2.43	0.48
1:D:328:LEU:HD23	1:D:432:ILE:HG21	1.94	0.48
1:D:504:ASN:HB2	1:D:505:LYS:NZ	2.28	0.48
1:B:297:PRO:HB3	1:B:320:ASP:OD2	2.13	0.48
1:D:88:ASN:HD21	1:D:104:ASN:HA	1.79	0.48
1:A:95:GLN:NE2	1:A:100:VAL:HG22	2.28	0.48
1:A:183:PRO:HB2	1:A:203:ILE:CG2	2.43	0.48
1:A:45:PHE:HE2	1:B:10:THR:HG21	1.78	0.48
1:A:47:VAL:HG22	1:B:14:VAL:CA	2.43	0.48
1:C:272:HIS:HD2	1:C:274:GLU:HB2	1.77	0.48
1:D:343:PRO:HD2	1:D:388:TYR:OH	2.13	0.48
1:A:39:LYS:HD2	1:A:45:PHE:CE1	2.48	0.48
1:A:452:MET:HG3	1:A:487:TRP:CH2	2.49	0.48
1:C:334:GLN:HB2	3:C:980:HOH:O	2.14	0.48
1:C:328:LEU:HD22	1:C:432:ILE:HG21	1.95	0.48
1:D:261:MET:H	1:D:307:GLN:NE2	2.11	0.48
1:A:151:ASN:ND2	1:A:200:ASN:HD21	2.12	0.48
1:A:308:LEU:O	1:A:312:GLU:HG2	2.13	0.48
1:A:494:ARG:CG	1:A:495:PRO:HD2	2.43	0.48
1:C:257:VAL:HG13	1:C:258:ASN:N	2.29	0.48
1:D:193:ALA:C	1:D:195:GLN:H	2.17	0.48
1:C:533:LEU:HD22	1:D:494:ARG:NH1	2.28	0.48
1:B:435:VAL:O	1:B:436:CYS:HB3	2.14	0.48
1:C:343:PRO:HD2	1:C:388:TYR:OH	2.14	0.48
1:C:376:VAL:HG22	1:C:501:ASN:HB3	1.96	0.48
1:D:441:LEU:HD12	3:D:946:HOH:O	2.14	0.48
1:A:225:ARG:HG3	3:A:882:HOH:O	2.13	0.48
1:B:407:PRO:HB3	1:D:344:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ARG:HD2	3:B:851:HOH:O	2.14	0.48
1:D:24:ASN:OD1	1:D:61:LYS:HB2	2.14	0.48
1:A:131:ASN:HD22	1:A:131:ASN:N	2.10	0.48
1:A:299:ASN:N	1:A:299:ASN:HD22	2.11	0.48
1:D:180:LYS:HD2	3:D:928:HOH:O	2.13	0.48
1:D:325:GLN:CA	1:D:325:GLN:HE21	2.17	0.48
1:D:64:GLU:O	1:D:65:LYS:HE3	2.14	0.48
1:A:112:CYS:HA	1:B:386:ILE:HG21	1.96	0.47
1:A:122:GLU:OE1	1:A:122:GLU:N	2.48	0.47
1:B:257:VAL:HG13	1:B:272:HIS:CD2	2.49	0.47
1:D:247:THR:CG2	1:D:297:PRO:HG2	2.43	0.47
1:B:20:THR:CG2	1:B:21:TYR:N	2.77	0.47
1:B:229:ASN:O	1:B:233:GLU:HG3	2.15	0.47
1:C:394:LYS:HB3	1:C:394:LYS:HZ3	1.78	0.47
1:C:386:ILE:HG21	1:D:112:CYS:HA	1.95	0.47
1:D:137:VAL:HG13	3:D:696:HOH:O	2.14	0.47
1:D:71:ILE:HD13	1:D:243:TRP:HE3	1.79	0.47
1:D:261:MET:HE1	1:D:311:HIS:HB2	1.95	0.47
1:D:360:LEU:O	1:D:360:LEU:HD13	2.14	0.47
1:C:412:LYS:HE2	1:C:414:ALA:HB2	1.96	0.47
1:D:220:LEU:O	1:D:224:ARG:HG3	2.14	0.47
1:B:500:VAL:O	1:B:500:VAL:HG13	2.13	0.47
1:D:248:GLU:H	1:D:298:GLN:NE2	2.12	0.47
1:D:254:SER:HB2	1:D:257:VAL:HB	1.97	0.47
1:D:266:GLN:NE2	1:D:270:ASN:HD21	2.12	0.47
1:B:224:ARG:HD2	1:B:287:LEU:HD23	1.96	0.47
1:C:251:VAL:HG21	1:C:274:GLU:O	2.14	0.47
1:C:372:SER:HB3	1:C:490:ALA:HB2	1.96	0.47
1:D:200:ASN:HD22	1:D:200:ASN:C	2.16	0.47
1:D:504:ASN:ND2	3:D:827:HOH:O	2.47	0.47
1:D:253:VAL:O	1:D:253:VAL:HG13	2.15	0.47
1:B:352:LEU:HD22	1:B:352:LEU:C	2.34	0.47
1:C:229:ASN:HB3	1:C:233:GLU:OE1	2.14	0.47
1:C:481:LEU:HA	3:C:852:HOH:O	2.15	0.47
1:A:39:LYS:HB2	1:A:45:PHE:CE1	2.49	0.47
1:B:332:LEU:O	1:B:335:PHE:HB3	2.15	0.47
1:C:342:LYS:HB2	1:C:387:LEU:HG	1.97	0.47
1:D:325:GLN:HG2	1:D:414:ALA:HB1	1.96	0.47
1:C:445:LEU:HG	1:C:487:TRP:CD1	2.50	0.47
1:D:71:ILE:HG21	1:D:243:TRP:CE3	2.49	0.47
1:C:200:ASN:HD22	1:C:200:ASN:C	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:HIS:CD2	1:C:274:GLU:HB2	2.49	0.47
1:C:296:SER:C	1:C:320:ASP:H	2.18	0.47
2:D:680:NAD:O2N	2:D:680:NAD:N7N	2.48	0.47
1:D:231:LYS:HE2	1:D:239:VAL:CG1	2.45	0.47
1:A:151:ASN:HB2	1:A:180:LYS:CE	2.45	0.46
1:A:345:SER:HA	1:A:397:ASP:O	2.15	0.46
1:B:193:ALA:H	1:B:196:ASP:HB2	1.79	0.46
1:B:489:LYS:O	1:B:491:PRO:HD3	2.15	0.46
1:A:476:ASN:HB3	3:A:875:HOH:O	2.15	0.46
1:C:257:VAL:HG13	1:C:258:ASN:H	1.79	0.46
1:D:22:LYS:HB2	1:D:25:GLU:HB3	1.97	0.46
1:A:84:SER:HB3	1:B:423:MET:HE3	1.96	0.46
1:B:131:ASN:ND2	1:B:131:ASN:C	2.69	0.46
1:B:198:ARG:NH2	1:B:355:ASN:HD21	2.12	0.46
1:B:38:THR:HG22	1:B:39:LYS:N	2.30	0.46
1:A:54:TYR:CE2	1:B:532:LEU:HD23	2.50	0.46
1:D:167:ASP:O	1:D:171:ARG:HG3	2.15	0.46
1:D:262:GLU:HA	1:D:262:GLU:OE2	2.16	0.46
1:B:216:LYS:O	1:B:219:HIS:HB2	2.15	0.46
1:C:217:TRP:O	1:C:220:LEU:HB3	2.14	0.46
1:A:131:ASN:HD22	1:A:131:ASN:H	1.63	0.46
1:B:73:LEU:HD23	1:B:181:PRO:HB3	1.98	0.46
1:D:151:ASN:C	1:D:151:ASN:HD22	2.17	0.46
1:A:206:ASP:OD1	1:A:208:LYS:N	2.48	0.46
1:D:206:ASP:N	1:D:210:ASN:O	2.38	0.46
1:D:37:VAL:HG22	1:D:47:VAL:HG22	1.97	0.46
1:A:453:THR:O	1:A:457:THR:HG23	2.15	0.46
1:A:516:LEU:C	1:A:516:LEU:HD12	2.35	0.46
1:A:45:PHE:HB2	1:B:12:VAL:HG22	1.98	0.46
1:B:10:THR:N	3:B:917:HOH:O	2.48	0.46
1:A:192:ALA:O	1:A:193:ALA:C	2.53	0.46
1:B:248:GLU:HB2	1:B:298:GLN:HG2	1.97	0.46
1:B:39:LYS:HE2	1:B:43:GLY:HA2	1.98	0.46
1:C:262:GLU:HB2	3:C:830:HOH:O	2.16	0.46
1:A:299:ASN:HD22	1:A:299:ASN:H	1.64	0.46
1:A:494:ARG:HG3	1:A:495:PRO:HD2	1.98	0.46
1:D:121:ALA:HB3	1:D:122:GLU:OE2	2.16	0.46
1:D:153:ASP:OD2	1:D:155:TYR:HB3	2.16	0.46
1:D:38:THR:HG23	1:D:38:THR:O	2.16	0.46
1:D:40:THR:CG2	1:D:44:ARG:H	2.28	0.46
1:B:21:TYR:CE1	1:B:26:LEU:HD23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:LYS:C	1:B:491:PRO:HD3	2.36	0.45
1:C:473:LYS:O	1:C:473:LYS:HG2	2.16	0.45
1:D:329:LYS:NZ	1:D:348:SER:HB2	2.31	0.45
1:D:452:MET:HG3	1:D:487:TRP:CH2	2.50	0.45
1:B:250:TYR:HD1	3:B:858:HOH:O	1.98	0.45
1:B:453:THR:O	1:B:457:THR:HG23	2.16	0.45
1:C:363:PRO:HA	1:C:366:PHE:HB3	1.98	0.45
1:C:413:VAL:HG22	1:C:435:VAL:HG22	1.97	0.45
1:D:150:ASN:HA	1:D:200:ASN:ND2	2.31	0.45
1:A:131:ASN:ND2	1:A:131:ASN:H	2.14	0.45
1:A:187:TYR:HA	1:A:188:PRO:HD2	1.79	0.45
1:A:389:ASN:OD1	1:A:392:LEU:HD23	2.16	0.45
1:A:404:TYR:OH	1:A:406:LYS:HG2	2.17	0.45
1:B:220:LEU:O	1:B:220:LEU:HD23	2.16	0.45
1:B:246:ASN:HB3	3:B:987:HOH:O	2.15	0.45
1:B:18:LYS:O	1:B:28:THR:HA	2.16	0.45
1:A:147:TRP:HB3	1:A:184:SER:HB2	1.96	0.45
1:A:76:ASN:HB3	1:A:439:SER:OG	2.17	0.45
1:B:323:SER:N	1:B:489:LYS:HE3	2.17	0.45
1:D:71:ILE:HG21	1:D:243:TRP:CZ3	2.52	0.45
1:B:480:VAL:CG2	1:B:480:VAL:O	2.63	0.45
1:C:175:LYS:NZ	3:C:962:HOH:O	2.49	0.45
1:A:328:LEU:HD21	1:B:332:LEU:HD23	1.98	0.45
1:A:405:MET:O	1:A:408:VAL:HG23	2.16	0.45
1:B:115:LEU:HG	1:B:511:GLU:HG3	1.97	0.45
1:C:198:ARG:NH2	1:C:355:ASN:ND2	2.65	0.45
1:C:293:ILE:HA	1:C:317:ALA:O	2.17	0.45
1:A:248:GLU:OE2	1:A:277:PRO:HD2	2.17	0.45
1:B:139:PRO:HA	1:B:142:PHE:CE2	2.52	0.45
1:B:198:ARG:HH22	1:B:355:ASN:ND2	2.15	0.45
1:D:445:LEU:HD23	1:D:445:LEU:C	2.37	0.45
1:A:208:LYS:HB2	1:A:210:ASN:OD1	2.17	0.45
1:B:192:ALA:O	1:B:193:ALA:HB3	2.17	0.45
1:B:206:ASP:OD1	1:B:209:GLY:N	2.49	0.45
1:C:364:LYS:HB2	1:C:365:GLN:NE2	2.31	0.45
1:B:195:GLN:N	1:B:195:GLN:NE2	2.65	0.45
1:B:348:SER:C	1:B:349:TYR:CD1	2.90	0.45
1:B:452:MET:HG3	1:B:487:TRP:CH2	2.52	0.45
1:C:371:ILE:HG22	1:C:372:SER:N	2.31	0.45
1:C:500:VAL:HG21	1:D:527:ARG:HE	1.79	0.45
1:D:121:ALA:N	3:D:740:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:TRP:O	1:D:221:GLN:HG3	2.17	0.45
1:D:412:LYS:HE3	1:D:438:ASP:CG	2.38	0.45
1:A:225:ARG:HH11	1:A:228:GLN:NE2	2.14	0.45
1:A:489:LYS:HD3	3:A:986:HOH:O	2.16	0.45
1:B:322:LYS:HA	1:B:489:LYS:CG	2.32	0.45
1:B:315:PHE:CD1	1:B:481:LEU:HD11	2.51	0.45
1:D:352:LEU:HA	1:D:412:LYS:CA	2.42	0.45
1:D:526:LEU:O	1:D:531:ARG:NE	2.43	0.45
1:B:218:THR:HG23	3:B:984:HOH:O	2.18	0.44
1:C:352:LEU:N	1:C:352:LEU:HD23	2.32	0.44
1:C:34:ASN:CG	1:C:35:ALA:H	2.20	0.44
1:C:55:VAL:CG2	1:C:464:VAL:HG11	2.47	0.44
1:D:261:MET:HE2	1:D:308:LEU:HA	1.99	0.44
1:A:299:ASN:N	1:A:299:ASN:ND2	2.65	0.44
1:A:65:LYS:NZ	3:A:996:HOH:O	2.50	0.44
1:B:272:HIS:HB3	1:B:275:ILE:HG12	1.99	0.44
1:C:22:LYS:HB3	1:C:22:LYS:NZ	2.32	0.44
1:C:315:PHE:CD1	1:C:481:LEU:HD11	2.53	0.44
1:C:319:ASP:HB2	1:C:490:ALA:O	2.18	0.44
1:D:190:PHE:O	1:D:249:ARG:HG3	2.17	0.44
1:C:148:ASP:HA	2:C:670:NAD:N3A	2.32	0.44
1:C:204:ASN:HB3	1:C:219:HIS:CE1	2.52	0.44
1:A:351:HIS:CD2	1:C:349:TYR:OH	2.69	0.44
1:A:282:ALA:HB3	1:A:305:LEU:HD21	1.99	0.44
1:A:452:MET:HG3	1:A:487:TRP:HH2	1.83	0.44
1:B:148:ASP:HA	2:B:660:NAD:N3A	2.32	0.44
1:C:335:PHE:HE2	1:D:327:LYS:HB3	1.82	0.44
1:A:352:LEU:HD22	1:A:352:LEU:O	2.18	0.44
1:B:180:LYS:HB3	3:B:732:HOH:O	2.17	0.44
1:B:198:ARG:NH2	1:B:355:ASN:ND2	2.66	0.44
1:D:505:LYS:HG2	3:D:950:HOH:O	2.15	0.44
1:A:224:ARG:NH1	1:A:287:LEU:HD13	2.33	0.44
1:A:322:LYS:NZ	3:A:847:HOH:O	2.50	0.44
1:B:501:ASN:HA	1:B:506:GLN:OE1	2.17	0.44
1:C:497:PHE:CD2	1:D:530:GLU:HG2	2.53	0.44
1:D:247:THR:HG21	1:D:297:PRO:HG2	1.99	0.44
1:C:335:PHE:CE2	1:D:327:LYS:HB3	2.53	0.44
1:D:523:GLN:HA	1:D:523:GLN:HE21	1.83	0.44
1:B:349:TYR:N	1:B:349:TYR:CD1	2.85	0.44
1:C:296:SER:O	1:C:319:ASP:HA	2.17	0.44
1:C:372:SER:O	1:C:489:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:LEU:HB3	1:D:135:PRO:HD2	1.99	0.44
1:D:308:LEU:HD22	1:D:308:LEU:O	2.18	0.44
1:D:315:PHE:CZ	1:D:481:LEU:HD21	2.52	0.44
1:A:234:ASN:HB2	1:A:236:LEU:HG	2.00	0.44
1:C:503:LEU:HA	1:C:506:GLN:OE1	2.18	0.44
1:A:158:MET:HE2	1:A:176:MET:HG3	1.98	0.43
1:A:246:ASN:HD22	1:A:359:ASN:HD22	1.66	0.43
1:C:445:LEU:C	1:C:445:LEU:HD23	2.38	0.43
1:D:96:THR:HG21	1:D:101:LYS:HD2	1.99	0.43
1:D:347:ALA:HB1	1:D:349:TYR:CE2	2.52	0.43
1:B:348:SER:CB	1:B:416:ASP:OD2	2.66	0.43
1:B:71:ILE:HG21	1:B:243:TRP:CZ3	2.53	0.43
1:D:119:ILE:HA	1:D:124:ASN:O	2.18	0.43
1:D:315:PHE:CD1	1:D:481:LEU:HD11	2.53	0.43
1:A:117:LEU:HB3	3:A:798:HOH:O	2.18	0.43
1:A:172:LEU:O	1:A:176:MET:HG2	2.18	0.43
1:A:134:LEU:HD11	1:A:517:LEU:HB2	2.00	0.43
1:B:352:LEU:HD21	1:B:356:ASP:O	2.18	0.43
1:B:91:ASN:HB3	3:B:752:HOH:O	2.17	0.43
1:C:259:ASP:N	1:C:259:ASP:OD2	2.51	0.43
1:D:22:LYS:HE3	1:D:27:LEU:CD1	2.40	0.43
1:D:272:HIS:CD2	1:D:274:GLU:H	2.36	0.43
1:D:352:LEU:HB3	1:D:412:LYS:CB	2.46	0.43
1:C:112:CYS:HB3	1:D:387:LEU:HD11	1.99	0.43
1:B:462:LYS:HD2	1:B:472:GLY:O	2.17	0.43
1:B:310:GLU:HA	1:B:479:PRO:HG3	2.00	0.43
1:C:358:TYR:HB2	1:C:404:TYR:CE1	2.54	0.43
1:D:465:ASP:HB3	1:D:468:LYS:HB3	2.00	0.43
1:A:381:ILE:HG23	1:A:388:TYR:CB	2.49	0.43
1:B:117:LEU:HD21	1:B:133:LEU:CD2	2.48	0.43
1:B:183:PRO:HB2	1:B:203:ILE:CG2	2.48	0.43
1:B:355:ASN:HB3	2:B:660:NAD:O1A	2.18	0.43
1:D:295:GLY:CA	1:D:321:LEU:HD13	2.48	0.43
1:D:447:ILE:O	1:D:451:VAL:HG23	2.18	0.43
1:B:333:ALA:O	1:B:337:VAL:HG22	2.18	0.43
1:C:22:LYS:HB3	1:C:25:GLU:HB2	2.00	0.43
1:C:350:ASN:HB3	1:C:414:ALA:HA	2.00	0.43
1:C:478:TYR:CE2	1:C:494:ARG:HG2	2.53	0.43
1:A:148:ASP:HA	2:A:650:NAD:N3A	2.33	0.43
1:B:352:LEU:CD1	1:B:352:LEU:N	2.82	0.43
1:C:174:ALA:HB2	3:C:933:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:GLY:H	1:C:259:ASP:CG	2.22	0.43
1:C:257:VAL:HG21	1:C:272:HIS:NE2	2.33	0.43
1:C:449:LEU:HD21	1:C:487:TRP:HB2	2.01	0.43
1:D:266:GLN:HE21	1:D:270:ASN:ND2	2.16	0.43
1:D:40:THR:HG21	1:D:44:ARG:HH12	1.75	0.43
1:A:224:ARG:O	1:A:228:GLN:HG3	2.19	0.43
1:A:286:ILE:HG23	1:A:314:THR:CG2	2.48	0.43
1:B:109:MET:HE3	1:B:486:TYR:CZ	2.54	0.43
1:B:266:GLN:HE21	1:B:270:ASN:ND2	2.14	0.43
1:C:282:ALA:O	1:C:286:ILE:HG13	2.19	0.43
1:D:200:ASN:C	1:D:200:ASN:ND2	2.71	0.43
1:D:352:LEU:HD22	1:D:354:ASN:OD1	2.18	0.43
1:A:501:ASN:ND2	3:A:795:HOH:O	2.51	0.43
1:A:134:LEU:HD11	1:A:517:LEU:CB	2.49	0.43
1:C:272:HIS:HD2	1:C:274:GLU:H	1.62	0.43
1:C:115:LEU:HD22	1:C:511:GLU:HG2	1.99	0.43
1:D:286:ILE:HG23	1:D:314:THR:OG1	2.19	0.43
1:D:452:MET:HG3	1:D:487:TRP:HH2	1.84	0.43
1:D:497:PHE:N	1:D:497:PHE:CD1	2.87	0.43
1:A:286:ILE:HG21	1:A:308:LEU:HD22	2.01	0.43
1:B:195:GLN:HG2	1:B:246:ASN:ND2	2.34	0.43
1:C:14:VAL:O	1:C:16:THR:HG22	2.18	0.43
1:C:483:PHE:HA	1:D:531:ARG:NH2	2.34	0.43
1:C:476:ASN:HA	3:C:991:HOH:O	2.18	0.42
1:B:351:HIS:CD2	1:D:349:TYR:OH	2.72	0.42
1:D:90:HIS:HE1	3:D:790:HOH:O	2.01	0.42
1:B:40:THR:OG1	1:B:44:ARG:HB3	2.19	0.42
1:B:412:LYS:HE3	1:B:412:LYS:HB2	1.78	0.42
1:B:449:LEU:HD21	1:B:487:TRP:HB2	2.01	0.42
1:C:112:CYS:HB3	1:D:387:LEU:HD13	2.01	0.42
1:C:335:PHE:CE1	1:D:328:LEU:CD1	3.03	0.42
1:D:435:VAL:O	1:D:436:CYS:HB3	2.19	0.42
1:D:301:PHE:CD1	1:D:492:LEU:HD12	2.54	0.42
1:A:22:LYS:O	1:A:25:GLU:HB3	2.20	0.42
1:A:352:LEU:CD2	1:A:354:ASN:ND2	2.78	0.42
1:B:261:MET:O	1:B:265:LEU:HG	2.19	0.42
2:C:670:NAD:O2N	2:C:670:NAD:N7N	2.52	0.42
1:A:250:TYR:CE2	1:A:298:GLN:HA	2.54	0.42
1:A:406:LYS:HE2	3:A:699:HOH:O	2.19	0.42
1:A:448:ASP:HB3	1:A:487:TRP:CE2	2.54	0.42
1:B:42:SER:C	1:B:44:ARG:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ALA:HB3	1:C:365:GLN:CG	2.46	0.42
1:D:194:ASN:HB2	1:D:358:TYR:CE2	2.55	0.42
1:A:96:THR:HG21	1:A:101:LYS:HD2	2.02	0.42
1:A:220:LEU:CD2	1:A:280:ILE:HG23	2.47	0.42
1:A:418:TYR:O	1:A:429:ARG:HA	2.20	0.42
1:B:201:ASN:HD22	1:B:201:ASN:HA	1.65	0.42
1:B:189:ASP:O	1:B:249:ARG:HD2	2.19	0.42
1:C:112:CYS:HA	1:D:386:ILE:HG21	2.00	0.42
1:C:18:LYS:HA	1:C:29:LYS:CE	2.50	0.42
1:C:461:TYR:OH	1:D:533:LEU:N	2.52	0.42
1:C:495:PRO:HG2	1:C:496:GLY:H	1.82	0.42
1:D:155:TYR:O	1:D:159:GLN:HG3	2.20	0.42
1:D:187:TYR:CD1	1:D:277:PRO:HG3	2.55	0.42
1:A:110:THR:HA	1:A:130:PHE:CD2	2.54	0.42
1:A:137:VAL:HG12	3:A:651:HOH:O	2.19	0.42
1:A:407:PRO:HG3	1:C:395:LYS:CE	2.47	0.42
1:A:322:LYS:HZ1	1:A:506:GLN:HE22	1.66	0.42
1:B:139:PRO:HA	1:B:142:PHE:CD2	2.54	0.42
1:B:459:VAL:HB	1:B:477:PHE:CE1	2.54	0.42
1:C:322:LYS:HD2	1:C:327:LYS:HE2	2.00	0.42
1:C:76:ASN:HB3	1:C:439:SER:OG	2.19	0.42
1:A:187:TYR:CD1	1:A:213:THR:HG22	2.55	0.42
1:A:259:ASP:HA	1:A:303:PRO:HG2	2.02	0.42
1:A:354:ASN:HD22	1:A:354:ASN:C	2.22	0.42
1:B:405:MET:C	1:B:407:PRO:HD2	2.40	0.42
1:B:42:SER:O	1:B:44:ARG:N	2.50	0.42
1:B:310:GLU:CG	1:B:479:PRO:HG3	2.45	0.42
1:D:205:LEU:HA	1:D:210:ASN:O	2.20	0.42
1:D:239:VAL:O	1:D:290:VAL:HG13	2.20	0.42
1:B:350:ASN:HD21	1:B:402:ILE:HG12	1.85	0.42
1:C:200:ASN:C	1:C:200:ASN:ND2	2.73	0.42
1:A:405:MET:CE	1:C:397:ASP:HB3	2.50	0.42
1:B:26:LEU:HD22	1:B:27:LEU:N	2.34	0.42
1:B:454:GLU:OE1	1:B:458:ARG:NH2	2.53	0.42
1:C:69:MET:HE2	1:C:227:ILE:HG23	2.01	0.42
1:D:325:GLN:HG2	3:D:785:HOH:O	2.19	0.42
1:A:184:SER:OG	1:A:185:ILE:N	2.52	0.42
1:A:79:SER:HB3	3:A:740:HOH:O	2.19	0.42
1:A:90:HIS:HE1	3:A:784:HOH:O	2.02	0.42
1:B:183:PRO:HB2	1:B:203:ILE:HG23	2.02	0.42
1:A:389:ASN:ND2	1:A:392:LEU:HD21	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LYS:HB3	1:C:407:PRO:HD3	2.01	0.41
1:D:241:VAL:HG23	1:D:290:VAL:HG11	2.02	0.41
1:D:294:ASN:ND2	3:D:726:HOH:O	2.53	0.41
1:A:350:ASN:ND2	1:A:412:LYS:HE3	2.35	0.41
1:D:492:LEU:HD23	1:D:493:THR:N	2.35	0.41
1:A:185:ILE:HD11	1:A:223:ILE:CD1	2.51	0.41
1:A:247:THR:CG2	1:A:297:PRO:HG2	2.51	0.41
1:B:350:ASN:O	1:B:402:ILE:HA	2.20	0.41
1:C:22:LYS:HE3	3:C:773:HOH:O	2.20	0.41
1:C:398:HIS:CD2	1:C:398:HIS:N	2.89	0.41
1:C:462:LYS:HD2	1:C:473:LYS:HD3	2.02	0.41
1:D:266:GLN:HE21	1:D:270:ASN:HD21	1.69	0.41
1:D:384:ASN:O	1:D:388:TYR:HB2	2.21	0.41
1:B:27:LEU:HD22	1:B:27:LEU:N	2.35	0.41
1:D:352:LEU:HD11	1:D:357:GLY:CA	2.44	0.41
1:D:39:LYS:HE2	1:D:43:GLY:HA2	2.03	0.41
1:D:527:ARG:C	1:D:529:GLU:H	2.23	0.41
1:D:530:GLU:O	1:D:531:ARG:C	2.58	0.41
1:B:253:VAL:O	1:B:253:VAL:HG22	2.21	0.41
1:D:353:GLY:O	1:D:410:ASP:N	2.53	0.41
1:A:190:PHE:CE2	1:A:276:ALA:HB2	2.56	0.41
1:A:285:SER:HB3	1:A:290:VAL:CG2	2.51	0.41
1:A:343:PRO:HD2	1:A:388:TYR:OH	2.21	0.41
1:B:253:VAL:HA	1:B:258:ASN:OD1	2.21	0.41
1:B:408:VAL:HB	1:B:411:SER:O	2.21	0.41
1:C:254:SER:N	1:C:258:ASN:HD21	2.18	0.41
1:C:312:GLU:OE1	3:C:873:HOH:O	2.22	0.41
1:C:30:TYR:CD1	1:C:516:LEU:HG	2.56	0.41
1:C:532:LEU:O	1:C:533:LEU:OXT	2.39	0.41
1:C:193:ALA:C	1:C:195:GLN:H	2.23	0.41
1:C:327:LYS:O	1:C:331:VAL:HG23	2.21	0.41
1:C:356:ASP:O	1:C:360:LEU:HD23	2.20	0.41
1:C:477:PHE:HD1	3:C:991:HOH:O	2.04	0.41
1:D:530:GLU:O	1:D:532:LEU:N	2.53	0.41
1:A:528:PHE:C	1:A:530:GLU:H	2.24	0.41
1:A:532:LEU:HD23	1:B:54:TYR:CE2	2.56	0.41
1:C:298:GLN:H	1:C:298:GLN:HG3	1.45	0.41
1:D:323:SER:O	1:D:327:LYS:HG3	2.21	0.41
1:B:351:HIS:HD2	1:D:349:TYR:OH	2.03	0.41
1:D:494:ARG:HB3	1:D:495:PRO:HD2	2.03	0.41
1:A:65:LYS:HE2	1:A:141:ASP:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:NZ	3:A:806:HOH:O	2.48	0.41
1:A:285:SER:HB3	1:A:290:VAL:HG23	2.01	0.41
1:A:347:ALA:HB1	1:A:349:TYR:CE2	2.55	0.41
1:A:44:ARG:HH11	1:B:13:LYS:CB	2.34	0.41
1:B:212:THR:HG22	1:B:214:ARG:N	2.27	0.41
1:B:248:GLU:N	1:B:298:GLN:HG2	2.27	0.41
1:C:150:ASN:HB2	1:C:198:ARG:HG2	2.03	0.41
1:C:362:ALA:HA	1:C:363:PRO:HD2	1.90	0.41
1:D:289:GLY:HA2	1:D:314:THR:HG22	2.01	0.41
1:A:256:GLY:C	1:A:263:ASN:HD22	2.24	0.41
1:B:516:LEU:C	1:B:516:LEU:HD12	2.41	0.41
1:C:134:LEU:HD21	1:C:518:ILE:CG2	2.51	0.41
1:C:249:ARG:HG3	1:C:249:ARG:HH21	1.86	0.41
1:C:349:TYR:CD1	1:C:401:VAL:HB	2.56	0.41
1:D:261:MET:HE3	1:D:307:GLN:HG2	2.03	0.41
1:A:69:MET:HE1	1:A:227:ILE:CA	2.30	0.41
1:B:423:MET:CE	1:B:424:LEU:HD22	2.50	0.41
1:C:112:CYS:SG	1:D:387:LEU:HD11	2.61	0.41
1:D:437:GLU:H	1:D:437:GLU:HG2	1.44	0.41
1:D:41:ALA:C	1:D:43:GLY:H	2.24	0.41
1:A:394:LYS:O	1:A:394:LYS:CG	2.69	0.40
1:B:404:TYR:OH	1:B:406:LYS:HB2	2.21	0.40
1:A:533:LEU:HD21	1:B:463:LYS:HE2	2.03	0.40
1:B:494:ARG:HB2	1:B:497:PHE:CD1	2.56	0.40
1:C:69:MET:CE	1:C:227:ILE:HA	2.51	0.40
1:D:297:PRO:HD3	1:D:320:ASP:OD1	2.21	0.40
1:D:523:GLN:HA	1:D:523:GLN:NE2	2.36	0.40
1:D:527:ARG:C	1:D:529:GLU:N	2.74	0.40
1:D:52:GLN:HG3	1:D:54:TYR:CE1	2.56	0.40
1:A:266:GLN:HA	1:A:269:LYS:HD2	2.04	0.40
1:A:403:LYS:HE3	1:C:401:VAL:HG22	2.04	0.40
1:B:325:GLN:CA	1:B:325:GLN:HE21	2.29	0.40
1:C:20:THR:HB	1:C:27:LEU:HB2	2.04	0.40
1:C:318:GLY:HA2	1:C:488:LEU:HD21	2.03	0.40
1:D:133:LEU:HD12	1:D:133:LEU:N	2.37	0.40
1:D:354:ASN:C	1:D:356:ASP:H	2.25	0.40
1:A:158:MET:HE1	1:A:176:MET:HG3	2.02	0.40
1:B:316:ILE:HD11	1:B:480:VAL:HG12	2.03	0.40
1:A:191:ILE:HG22	1:A:359:ASN:HD21	1.85	0.40
1:A:445:LEU:HG	1:A:487:TRP:CD1	2.56	0.40
1:B:135:PRO:HG2	1:B:458:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:PRO:HD2	3:B:811:HOH:O	2.21	0.40
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.96	0.40
1:D:462:LYS:HE2	1:D:472:GLY:O	2.22	0.40
1:A:102:GLN:NE2	3:A:811:HOH:O	2.46	0.40
1:A:478:TYR:HA	1:B:533:LEU:HD21	2.04	0.40
1:B:265:LEU:O	1:B:269:LYS:HG3	2.20	0.40
1:B:70:LEU:HD11	1:B:81:LEU:CD2	2.50	0.40
1:C:271:ASP:O	1:C:272:HIS:C	2.59	0.40
1:C:248:GLU:HB2	1:C:298:GLN:HE21	1.85	0.40
1:D:260:THR:HB	1:D:307:GLN:HE22	1.86	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%)	465 (93%)	28 (6%)	9 (2%)	8	2
1	B	485/533 (91%)	445 (92%)	32 (7%)	8 (2%)	9	2
1	C	513/533 (96%)	474 (92%)	27 (5%)	12 (2%)	6	1
1	D	481/533 (90%)	445 (92%)	28 (6%)	8 (2%)	9	2
All	All	1981/2132 (93%)	1829 (92%)	115 (6%)	37 (2%)	8	2

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ALA
1	A	211	VAL
1	A	319	ASP
1	A	495	PRO
1	B	192	ALA

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Mol	Chain	Res	Type
1	B	319	ASP
1	C	193	ALA
1	D	319	ASP
1	B	191	ILE
1	C	199	ALA
1	C	319	ASP
1	D	531	ARG
1	A	195	GLN
1	B	193	ALA
1	B	347	ALA
1	C	22	LYS
1	C	189	ASP
1	C	194	ASN
1	C	272	HIS
1	C	322	LYS
1	D	23	ASP
1	D	470	ASP
1	B	320	ASP
1	A	212	THR
1	C	320	ASP
1	C	502	GLY
1	D	355	ASN
1	A	42	SER
1	A	479	PRO
1	A	502	GLY
1	D	194	ASN
1	B	502	GLY
1	B	346	ILE
1	C	495	PRO
1	D	346	ILE
1	D	479	PRO
1	C	464	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	446/471 (95%)	418 (94%)	28 (6%)	18 7
1	B	434/471 (92%)	412 (95%)	22 (5%)	24 11
1	C	458/471 (97%)	435 (95%)	23 (5%)	24 11
1	D	429/471 (91%)	403 (94%)	26 (6%)	18 7
All	All	1767/1884 (94%)	1668 (94%)	99 (6%)	21 9

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	47	VAL
1	A	65	LYS
1	A	79	SER
1	A	122	GLU
1	A	131	ASN
1	A	151	ASN
1	A	154	LEU
1	A	191	ILE
1	A	194	ASN
1	A	207	GLU
1	A	237	ASP
1	A	251	VAL
1	A	262	GLU
1	A	298	GLN
1	A	299	ASN
1	A	308	LEU
1	A	319	ASP
1	A	328	LEU
1	A	332	LEU
1	A	352	LEU
1	A	354	ASN
1	A	392	LEU
1	A	398	HIS
1	A	438	ASP
1	A	483	PHE
1	A	495	PRO
1	A	497	PHE
1	B	14	VAL
1	B	25	GLU
1	B	26	LEU
1	B	34	ASN
1	B	115	LEU

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Mol	Chain	Res	Type
1	B	131	ASN
1	B	194	ASN
1	B	195	GLN
1	B	200	ASN
1	B	201	ASN
1	B	205	LEU
1	B	207	GLU
1	B	218	THR
1	B	237	ASP
1	B	298	GLN
1	B	319	ASP
1	B	328	LEU
1	B	352	LEU
1	B	356	ASP
1	B	424	LEU
1	B	483	PHE
1	B	520	LEU
1	C	16	THR
1	C	22	LYS
1	C	62	LYS
1	C	200	ASN
1	C	201	ASN
1	C	236	LEU
1	C	238	LYS
1	C	251	VAL
1	C	258	ASN
1	C	298	GLN
1	C	308	LEU
1	C	334	GLN
1	C	364	LYS
1	C	387	LEU
1	C	394	LYS
1	C	397	ASP
1	C	398	HIS
1	C	440	LEU
1	C	441	LEU
1	C	483	PHE
1	C	488	LEU
1	C	516	LEU
1	C	523	GLN
1	D	24	ASN
1	D	25	GLU

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Mol	Chain	Res	Type
1	D	34	ASN
1	D	70	LEU
1	D	151	ASN
1	D	200	ASN
1	D	214	ARG
1	D	225	ARG
1	D	236	LEU
1	D	239	VAL
1	D	252	GLU
1	D	298	GLN
1	D	308	LEU
1	D	319	ASP
1	D	325	GLN
1	D	332	LEU
1	D	352	LEU
1	D	380	ILE
1	D	390	ASP
1	D	434	ASN
1	D	436	CYS
1	D	437	GLU
1	D	440	LEU
1	D	467	VAL
1	D	469	GLU
1	D	473	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	34	ASN
1	A	88	ASN
1	A	90	HIS
1	A	102	GLN
1	A	131	ASN
1	A	151	ASN
1	A	159	GLN
1	A	169	GLN
1	A	170	GLN
1	A	228	GLN
1	A	266	GLN
1	A	298	GLN
1	A	299	ASN

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Mol	Chain	Res	Type
1	A	325	GLN
1	A	351	HIS
1	A	354	ASN
1	A	359	ASN
1	A	398	HIS
1	A	428	ASN
1	A	433	HIS
1	A	506	GLN
1	A	512	ASN
1	B	34	ASN
1	B	95	GLN
1	B	102	GLN
1	B	131	ASN
1	B	159	GLN
1	B	169	GLN
1	B	170	GLN
1	B	195	GLN
1	B	200	ASN
1	B	201	ASN
1	B	228	GLN
1	B	229	ASN
1	B	263	ASN
1	B	270	ASN
1	B	298	GLN
1	B	325	GLN
1	B	351	HIS
1	B	501	ASN
1	B	506	GLN
1	B	512	ASN
1	B	523	GLN
1	C	24	ASN
1	C	77	ASN
1	C	90	HIS
1	C	150	ASN
1	C	151	ASN
1	C	169	GLN
1	C	170	GLN
1	C	195	GLN
1	C	200	ASN
1	C	201	ASN
1	C	221	GLN
1	C	228	GLN

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Mol	Chain	Res	Type
1	C	258	ASN
1	C	263	ASN
1	C	272	HIS
1	C	298	GLN
1	C	307	GLN
1	C	325	GLN
1	C	334	GLN
1	C	355	ASN
1	C	365	GLN
1	C	512	ASN
1	C	523	GLN
1	D	24	ASN
1	D	34	ASN
1	D	52	GLN
1	D	76	ASN
1	D	88	ASN
1	D	90	HIS
1	D	151	ASN
1	D	159	GLN
1	D	169	GLN
1	D	195	GLN
1	D	200	ASN
1	D	228	GLN
1	D	246	ASN
1	D	263	ASN
1	D	266	GLN
1	D	270	ASN
1	D	272	HIS
1	D	294	ASN
1	D	298	GLN
1	D	307	GLN
1	D	325	GLN
1	D	334	GLN
1	D	434	ASN
1	D	476	ASN
1	D	504	ASN
1	D	512	ASN
1	D	523	GLN

5.3.3 RNA

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 carbohydrates 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	$\#\|Z\| > 2$
2	NAD	A	650	-	42,48,48	2.08	7 (16%)	50,73,73	1.18	5 (10%)
2	NAD	C	670	-	42,48,48	1.91	7 (16%)	50,73,73	1.25	6 (12%)
2	NAD	B	660	-	42,48,48	2.25	9 (21%)	50,73,73	1.21	5 (10%)
2	NAD	D	680	-	42,48,48	2.03	8 (19%)	50,73,73	1.19	7 (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
2	NAD	A	650	-	-	1/26/62/62	0/5/5/5
2	NAD	C	670	-	-	3/26/62/62	0/5/5/5
2	NAD	B	660	-	-	2/26/62/62	0/5/5/5
2	NAD	D	680	-	-	4/26/62/62	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	660	NAD	C2N-N1N	8.00	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	650	NAD	C2N-N1N	7.04	1.43	1.35
2	C	670	NAD	C2N-N1N	6.25	1.42	1.35
2	B	660	NAD	C4N-C3N	6.23	1.50	1.39
2	D	680	NAD	C2N-N1N	6.19	1.42	1.35
2	A	650	NAD	C4N-C3N	6.14	1.49	1.39
2	D	680	NAD	C4N-C3N	6.08	1.49	1.39
2	C	670	NAD	C4N-C3N	5.50	1.48	1.39
2	D	680	NAD	C6N-N1N	4.64	1.46	1.35
2	A	650	NAD	C6N-N1N	4.55	1.46	1.35
2	C	670	NAD	C6N-N1N	4.49	1.46	1.35
2	B	660	NAD	C6N-N1N	4.12	1.45	1.35
2	B	660	NAD	C2A-N1A	3.93	1.41	1.33
2	B	660	NAD	C3N-C7N	3.83	1.56	1.50
2	A	650	NAD	C2A-N1A	3.67	1.40	1.33
2	B	660	NAD	C5N-C4N	3.64	1.46	1.38
2	D	680	NAD	C2A-N1A	3.61	1.40	1.33
2	C	670	NAD	C3N-C7N	3.31	1.55	1.50
2	A	650	NAD	C5N-C4N	3.21	1.45	1.38
2	D	680	NAD	C5N-C4N	3.17	1.45	1.38
2	C	670	NAD	C5N-C4N	3.11	1.45	1.38
2	D	680	NAD	C3N-C7N	2.94	1.55	1.50
2	C	670	NAD	C2A-N1A	2.92	1.39	1.33
2	A	650	NAD	C3N-C7N	2.66	1.54	1.50
2	B	660	NAD	C4A-N3A	2.63	1.39	1.35
2	D	680	NAD	C4A-N3A	2.55	1.39	1.35
2	A	650	NAD	C4A-N3A	2.54	1.39	1.35
2	D	680	NAD	O4B-C1B	-2.49	1.37	1.41
2	B	660	NAD	C2N-C3N	2.41	1.42	1.39
2	C	670	NAD	C4A-N3A	2.17	1.38	1.35
2	B	660	NAD	O4B-C1B	-2.01	1.38	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	660	NAD	C3N-C7N-N7N	3.82	122.34	117.75
2	A	650	NAD	C3N-C7N-N7N	3.53	121.99	117.75
2	C	670	NAD	O7N-C7N-N7N	-3.47	117.64	122.58
2	D	680	NAD	C3N-C7N-N7N	3.15	121.53	117.75
2	D	680	NAD	O7N-C7N-N7N	-3.13	118.12	122.58
2	A	650	NAD	O4B-C1B-C2B	-3.05	102.47	106.93
2	B	660	NAD	O4B-C1B-C2B	-3.05	102.47	106.93
2	C	670	NAD	C6N-N1N-C2N	-2.87	119.36	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	660	NAD	O7N-C7N-N7N	-2.84	118.54	122.58
2	C	670	NAD	O4B-C1B-C2B	-2.78	102.87	106.93
2	C	670	NAD	C3N-C7N-N7N	2.69	120.97	117.75
2	A	650	NAD	O7N-C7N-N7N	-2.64	118.82	122.58
2	C	670	NAD	C4A-C5A-N7A	2.62	112.13	109.40
2	A	650	NAD	C6N-N1N-C2N	-2.55	119.65	121.97
2	D	680	NAD	C1B-N9A-C4A	-2.48	122.28	126.64
2	A	650	NAD	C4A-C5A-N7A	2.44	111.94	109.40
2	D	680	NAD	O4B-C1B-C2B	-2.32	103.53	106.93
2	D	680	NAD	C5A-C6A-N6A	2.26	123.79	120.35
2	C	670	NAD	C1B-N9A-C4A	-2.20	122.77	126.64
2	D	680	NAD	O4D-C4D-C3D	2.14	109.35	105.11
2	B	660	NAD	C6N-N1N-C2N	-2.13	120.03	121.97
2	B	660	NAD	C5A-C6A-N6A	2.11	123.56	120.35
2	D	680	NAD	C4A-C5A-N7A	2.01	111.49	109.40

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	680	NAD	PN-O3-PA-O1A
2	A	650	NAD	O4B-C4B-C5B-O5B
2	C	670	NAD	PN-O3-PA-O1A
2	C	670	NAD	PN-O3-PA-O2A
2	D	680	NAD	PN-O3-PA-O2A
2	C	670	NAD	O4B-C4B-C5B-O5B
2	D	680	NAD	O4B-C4B-C5B-O5B
2	B	660	NAD	PA-O3-PN-O2N
2	D	680	NAD	C5D-O5D-PN-O1N
2	B	660	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

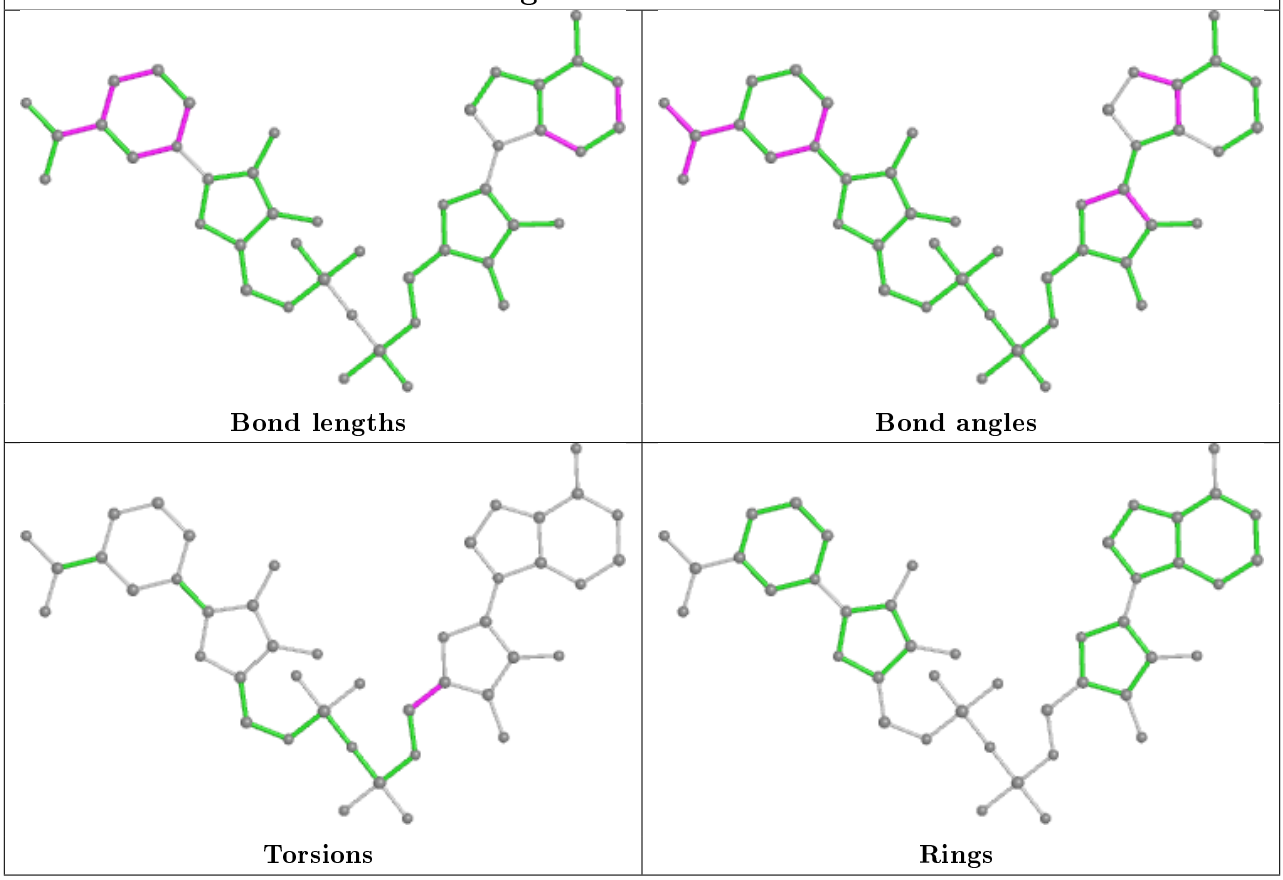
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	650	NAD	3	0
2	C	670	NAD	5	0
2	B	660	NAD	3	0
2	D	680	NAD	1	0

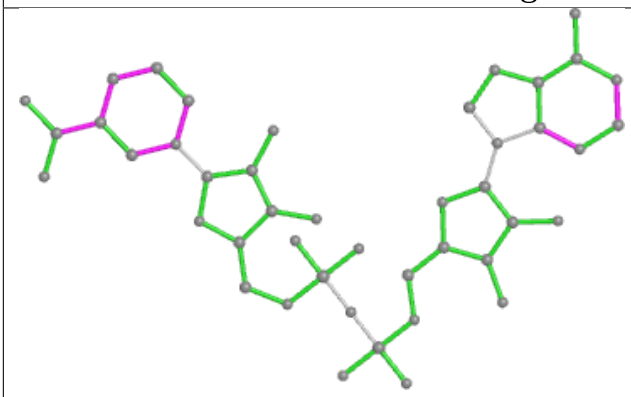
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

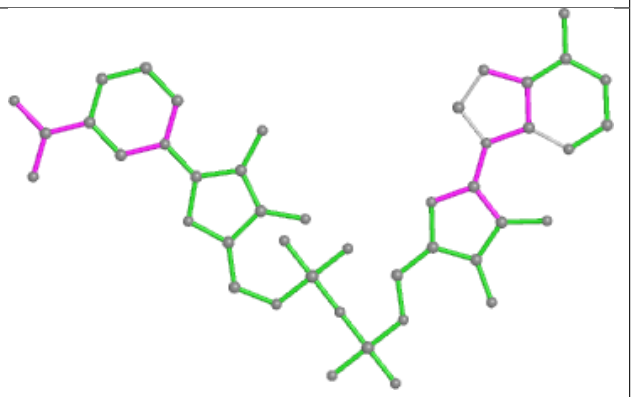
Ligand NAD A 650



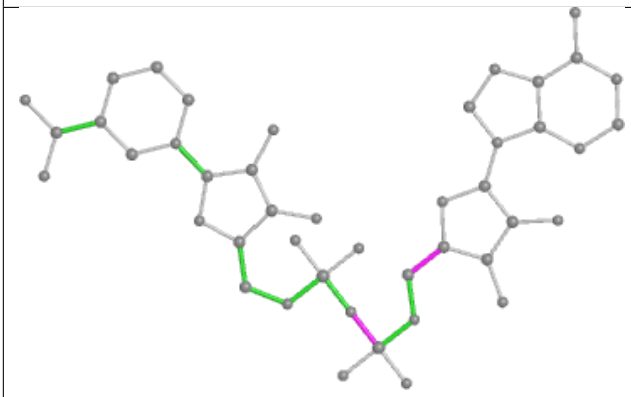
Ligand NAD C 670



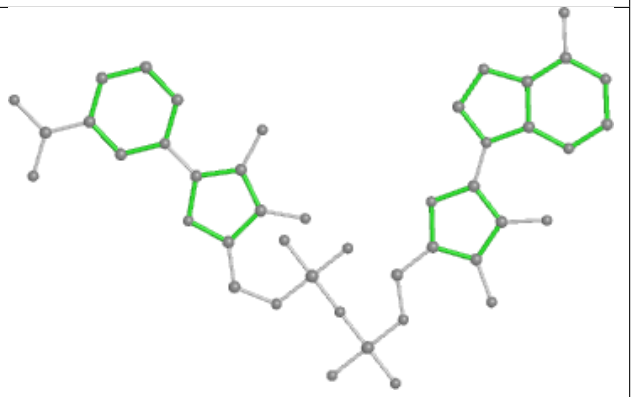
Bond lengths



Bond angles

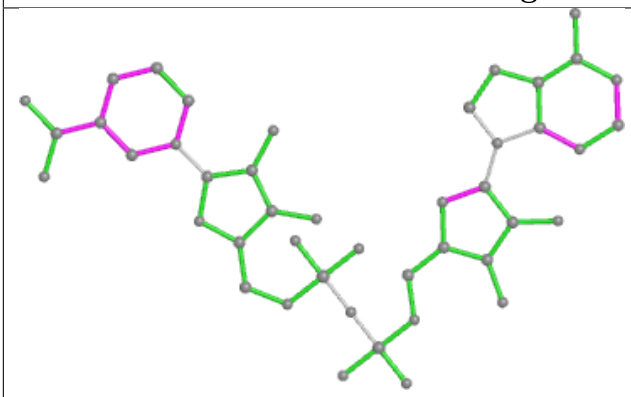


Torsions

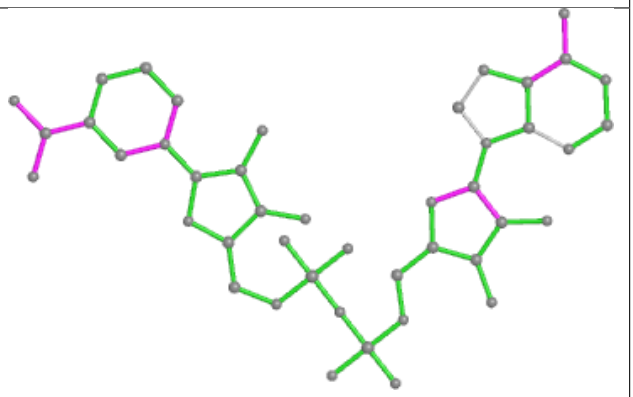


Rings

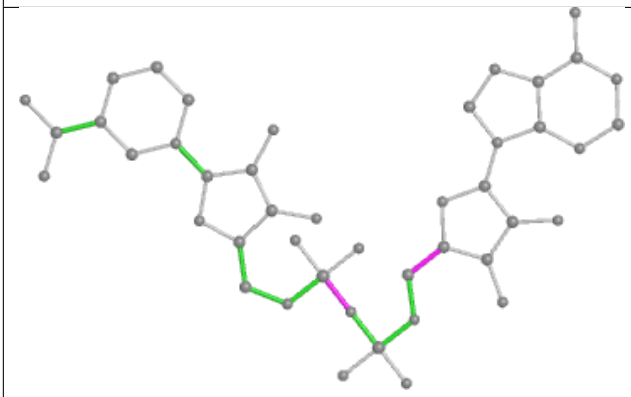
Ligand NAD B 660



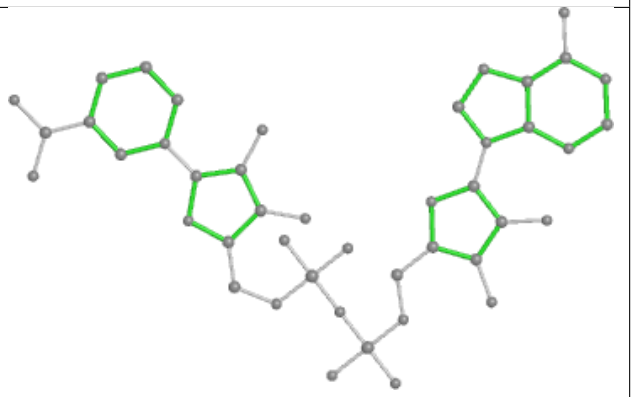
Bond lengths



Bond angles

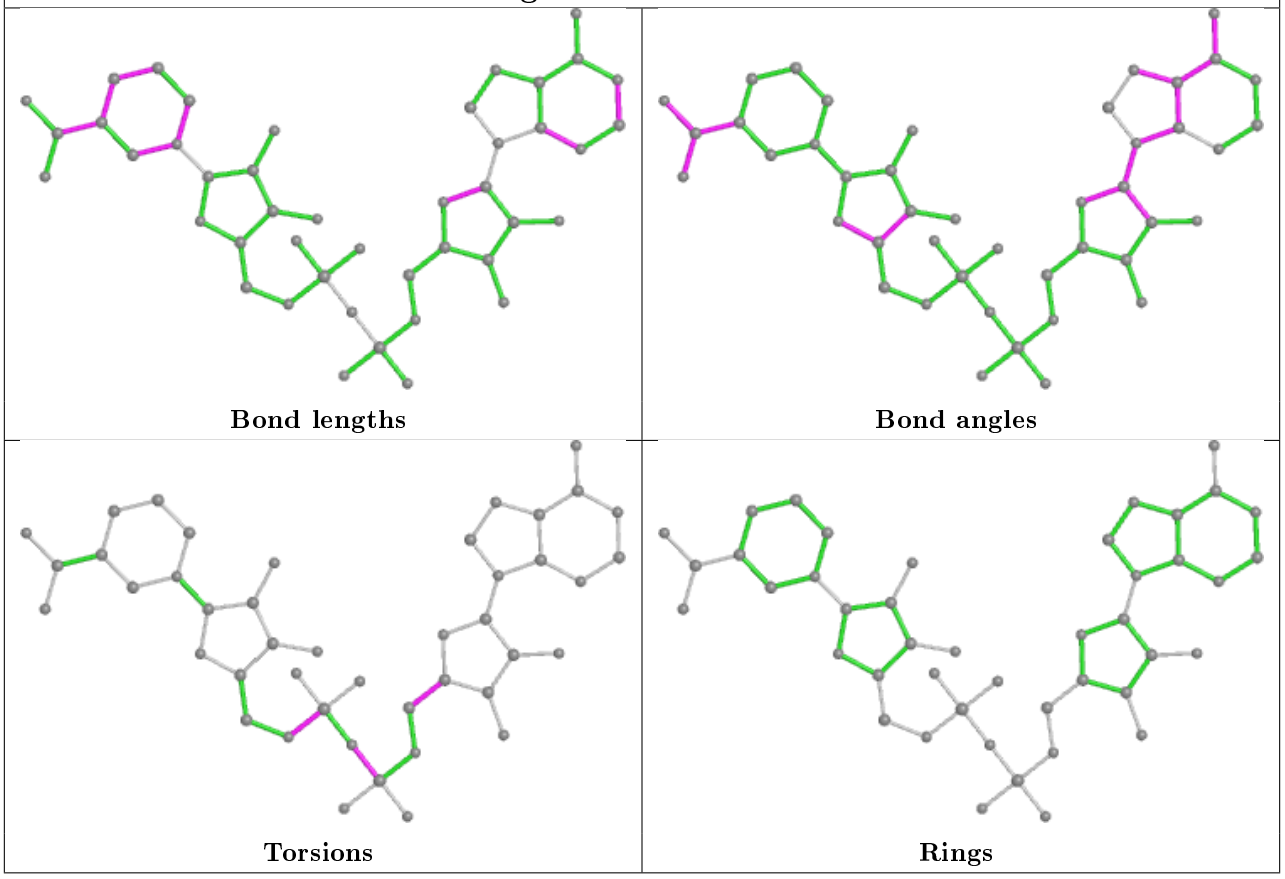


Torsions



Rings

Ligand NAD D 680



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.65	72 (14%)	2 4	24, 45, 85, 90	0
1	B	491/533 (92%)	0.71	77 (15%)	2 3	23, 45, 88, 90	0
1	C	517/533 (96%)	0.65	68 (13%)	3 5	22, 45, 86, 90	0
1	D	487/533 (91%)	0.61	66 (13%)	3 4	21, 41, 88, 90	0
All	All	2001/2132 (93%)	0.66	283 (14%)	2 4	21, 44, 87, 90	0

All (283) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	ALA	8.9
1	B	193	ALA	8.6
1	C	41	ALA	8.1
1	D	353	GLY	8.0
1	B	41	ALA	8.0
1	D	472	GLY	7.7
1	A	496	GLY	7.5
1	A	471	ALA	7.5
1	D	40	THR	7.3
1	B	404	TYR	6.9
1	B	396	VAL	6.7
1	B	40	THR	6.4
1	C	496	GLY	6.4
1	A	41	ALA	6.3
1	A	392	LEU	6.1
1	A	212	THR	6.1
1	B	394	LYS	6.1
1	D	381	ILE	6.1
1	B	42	SER	6.0
1	A	40	THR	6.0
1	D	471	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	42	SER	5.8
1	B	194	ASN	5.8
1	B	399	CYS	5.8
1	D	354	ASN	5.7
1	D	43	GLY	5.7
1	A	360	LEU	5.6
1	C	465	ASP	5.6
1	D	41	ALA	5.6
1	B	464	VAL	5.5
1	C	42	SER	5.5
1	D	352	LEU	5.4
1	D	194	ASN	5.4
1	D	358	TYR	5.2
1	C	497	PHE	5.2
1	A	497	PHE	5.1
1	A	358	TYR	4.9
1	B	472	GLY	4.9
1	D	473	LYS	4.9
1	C	533	LEU	4.9
1	C	363	PRO	4.8
1	C	495	PRO	4.8
1	D	499	PRO	4.8
1	B	393	GLY	4.8
1	C	390	ASP	4.8
1	A	194	ASN	4.7
1	C	374	SER	4.6
1	C	255	PRO	4.6
1	B	390	ASP	4.5
1	D	390	ASP	4.5
1	A	44	ARG	4.5
1	B	43	GLY	4.5
1	D	361	SER	4.4
1	D	193	ALA	4.3
1	D	197	GLU	4.3
1	C	372	SER	4.3
1	C	254	SER	4.2
1	B	398	HIS	4.2
1	B	407	PRO	4.2
1	C	40	THR	4.2
1	D	380	ILE	4.2
1	D	387	LEU	4.1
1	D	44	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	533	LEU	4.1
1	C	393	GLY	4.1
1	B	395	LYS	4.0
1	C	321	LEU	4.0
1	A	361	SER	4.0
1	A	498	HIS	4.0
1	D	360	LEU	4.0
1	D	42	SER	4.0
1	C	44	ARG	4.0
1	C	494	ARG	4.0
1	B	400	ILE	3.9
1	B	496	GLY	3.9
1	A	499	PRO	3.9
1	C	371	ILE	3.9
1	D	281	PHE	3.8
1	B	406	LYS	3.8
1	B	121	ALA	3.8
1	A	472	GLY	3.8
1	A	249	ARG	3.8
1	B	405	MET	3.8
1	C	23	ASP	3.8
1	D	389	ASN	3.8
1	A	70	LEU	3.8
1	A	211	VAL	3.7
1	A	391	LYS	3.7
1	B	280	ILE	3.7
1	B	392	LEU	3.7
1	A	398	HIS	3.7
1	A	397	ASP	3.7
1	A	390	ASP	3.6
1	B	210	ASN	3.5
1	B	71	ILE	3.5
1	C	24	ASN	3.5
1	A	400	ILE	3.5
1	C	395	LYS	3.5
1	C	280	ILE	3.5
1	D	207	GLU	3.5
1	B	38	THR	3.4
1	D	351	HIS	3.4
1	B	214	ARG	3.4
1	A	395	LYS	3.4
1	A	257	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	43	GLY	3.4
1	D	469	GLU	3.4
1	B	495	PRO	3.4
1	D	470	ASP	3.3
1	A	197	GLU	3.3
1	B	352	LEU	3.3
1	C	408	VAL	3.3
1	A	193	ALA	3.3
1	A	469	GLU	3.2
1	A	71	ILE	3.2
1	D	22	LYS	3.2
1	C	464	VAL	3.2
1	C	391	LYS	3.2
1	A	470	ASP	3.2
1	C	281	PHE	3.2
1	D	185	ILE	3.2
1	A	43	GLY	3.2
1	B	279	THR	3.2
1	B	208	LYS	3.2
1	A	210	ASN	3.2
1	A	533	LEU	3.1
1	D	121	ALA	3.1
1	C	373	LYS	3.1
1	C	22	LYS	3.1
1	A	254	SER	3.1
1	B	388	TYR	3.1
1	D	192	ALA	3.1
1	B	391	LYS	3.1
1	D	71	ILE	3.1
1	D	280	ILE	3.1
1	D	500	VAL	3.1
1	D	498	HIS	3.1
1	C	514	LEU	3.0
1	B	255	PRO	3.0
1	B	473	LYS	3.0
1	A	399	CYS	3.0
1	A	281	PHE	3.0
1	A	500	VAL	3.0
1	A	404	TYR	2.9
1	A	493	THR	2.9
1	B	498	HIS	2.9
1	C	320	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	70	LEU	2.9
1	B	197	GLU	2.9
1	B	389	ASN	2.9
1	A	39	LYS	2.9
1	D	39	LYS	2.9
1	B	61	LYS	2.9
1	C	361	SER	2.8
1	D	243	TRP	2.8
1	B	402	ILE	2.8
1	C	498	HIS	2.8
1	A	10	THR	2.8
1	C	479	PRO	2.8
1	D	253	VAL	2.8
1	B	351	HIS	2.8
1	A	501	ASN	2.8
1	D	481	LEU	2.8
1	D	255	PRO	2.8
1	A	467	VAL	2.8
1	D	344	VAL	2.8
1	A	38	THR	2.7
1	B	353	GLY	2.7
1	D	147	TRP	2.7
1	A	473	LYS	2.7
1	B	44	ARG	2.7
1	B	206	ASP	2.7
1	C	133	LEU	2.7
1	C	392	LEU	2.7
1	B	397	ASP	2.7
1	A	214	ARG	2.7
1	B	500	VAL	2.7
1	C	367	ARG	2.7
1	A	495	PRO	2.7
1	D	208	LYS	2.7
1	D	242	LEU	2.7
1	B	281	PHE	2.6
1	A	242	LEU	2.6
1	A	276	ALA	2.6
1	B	344	VAL	2.6
1	D	388	TYR	2.6
1	A	406	LYS	2.6
1	C	277	PRO	2.6
1	A	408	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	279	THR	2.6
1	B	242	LEU	2.6
1	B	122	GLU	2.6
1	B	514	LEU	2.6
1	B	403	LYS	2.6
1	B	123	GLY	2.6
1	C	256	GLY	2.6
1	C	21	TYR	2.5
1	D	51	VAL	2.5
1	B	81	LEU	2.5
1	C	71	ILE	2.5
1	B	401	VAL	2.5
1	B	39	LYS	2.5
1	C	349	TYR	2.5
1	C	260	THR	2.5
1	B	249	ARG	2.5
1	D	355	ASN	2.5
1	C	477	PHE	2.5
1	D	254	SER	2.5
1	B	348	SER	2.4
1	C	375	SER	2.4
1	D	38	THR	2.4
1	A	514	LEU	2.4
1	A	517	LEU	2.4
1	C	121	ALA	2.4
1	C	315	PHE	2.4
1	B	350	ASN	2.4
1	C	197	GLU	2.4
1	D	209	GLY	2.4
1	C	364	LYS	2.4
1	A	263	ASN	2.4
1	A	277	PRO	2.4
1	D	210	ASN	2.4
1	B	209	GLY	2.4
1	C	278	SER	2.3
1	D	347	ALA	2.3
1	C	185	ILE	2.3
1	B	133	LEU	2.3
1	C	500	VAL	2.3
1	C	478	TYR	2.3
1	D	212	THR	2.3
1	B	533	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	513	PHE	2.3
1	D	252	GLU	2.3
1	C	362	ALA	2.3
1	B	300	THR	2.2
1	C	300	THR	2.2
1	C	499	PRO	2.2
1	A	243	TRP	2.2
1	D	214	ARG	2.2
1	A	513	PHE	2.2
1	D	382	ALA	2.2
1	B	408	VAL	2.2
1	B	346	ILE	2.2
1	D	477	PHE	2.2
1	D	497	PHE	2.2
1	C	207	GLU	2.2
1	A	280	ILE	2.2
1	B	409	GLY	2.2
1	C	378	ASP	2.2
1	C	61	LYS	2.2
1	B	212	THR	2.1
1	C	279	THR	2.1
1	D	10	THR	2.1
1	A	259	ASP	2.1
1	B	70	LEU	2.1
1	A	252	GLU	2.1
1	B	243	TRP	2.1
1	C	394	LYS	2.1
1	A	270	ASN	2.1
1	A	359	ASN	2.1
1	C	194	ASN	2.1
1	A	352	LEU	2.1
1	A	122	GLU	2.1
1	C	122	GLU	2.1
1	C	17	ASP	2.1
1	A	207	GLU	2.1
1	A	255	PRO	2.1
1	D	122	GLU	2.1
1	A	147	TRP	2.1
1	B	278	SER	2.1
1	B	356	ASP	2.1
1	D	311	HIS	2.1
1	D	359	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	302	VAL	2.0
1	A	394	LYS	2.0
1	C	209	GLY	2.0
1	B	205	LEU	2.0
1	A	262	GLU	2.0
1	B	354	ASN	2.0
1	C	243	TRP	2.0
1	B	195	GLN	2.0
1	B	196	ASP	2.0
1	A	389	ASN	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 carbohydrates in this entry.

6.4 Ligands (i)

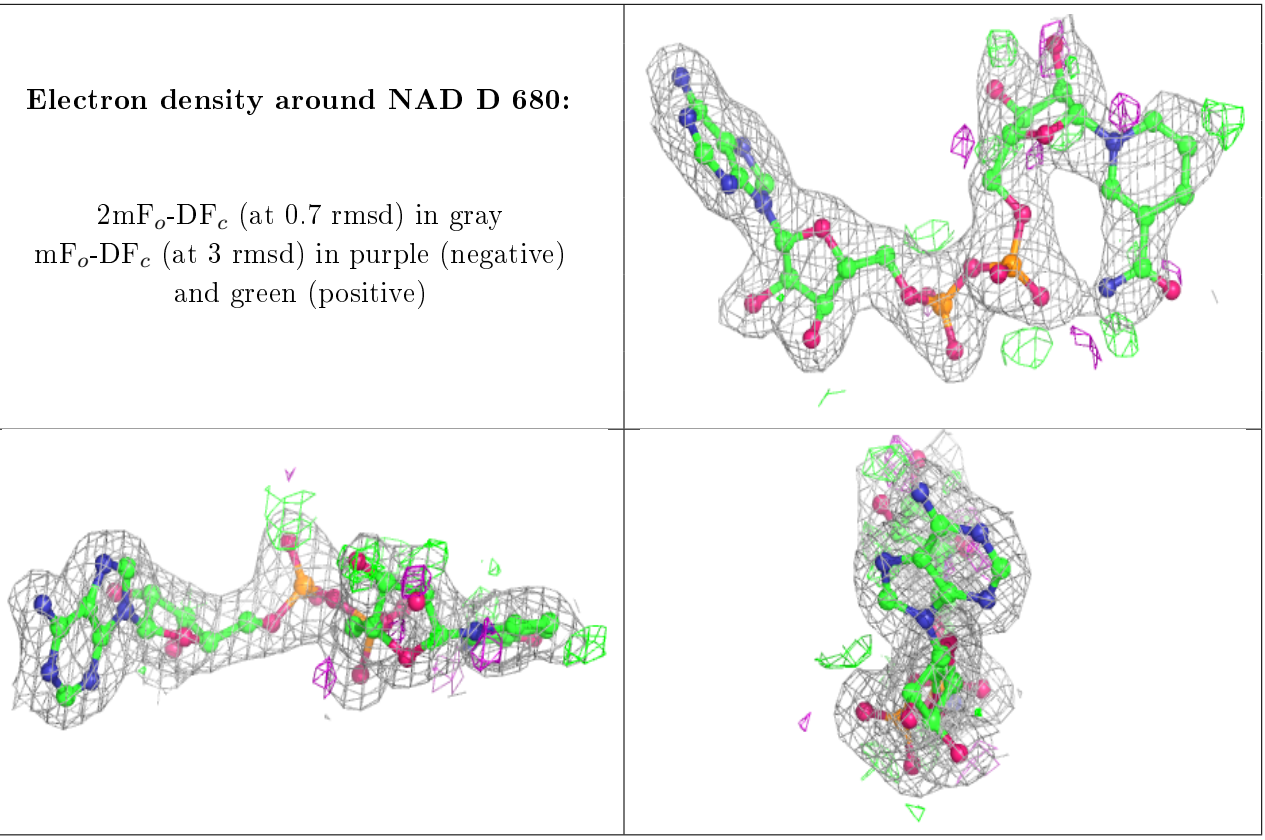
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	D	680	44/44	0.95	0.13	26,35,70,75	0
2	NAD	A	650	44/44	0.96	0.14	32,40,65,68	0
2	NAD	B	660	44/44	0.97	0.12	29,40,56,57	0
2	NAD	C	670	44/44	0.97	0.14	29,34,65,70	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.

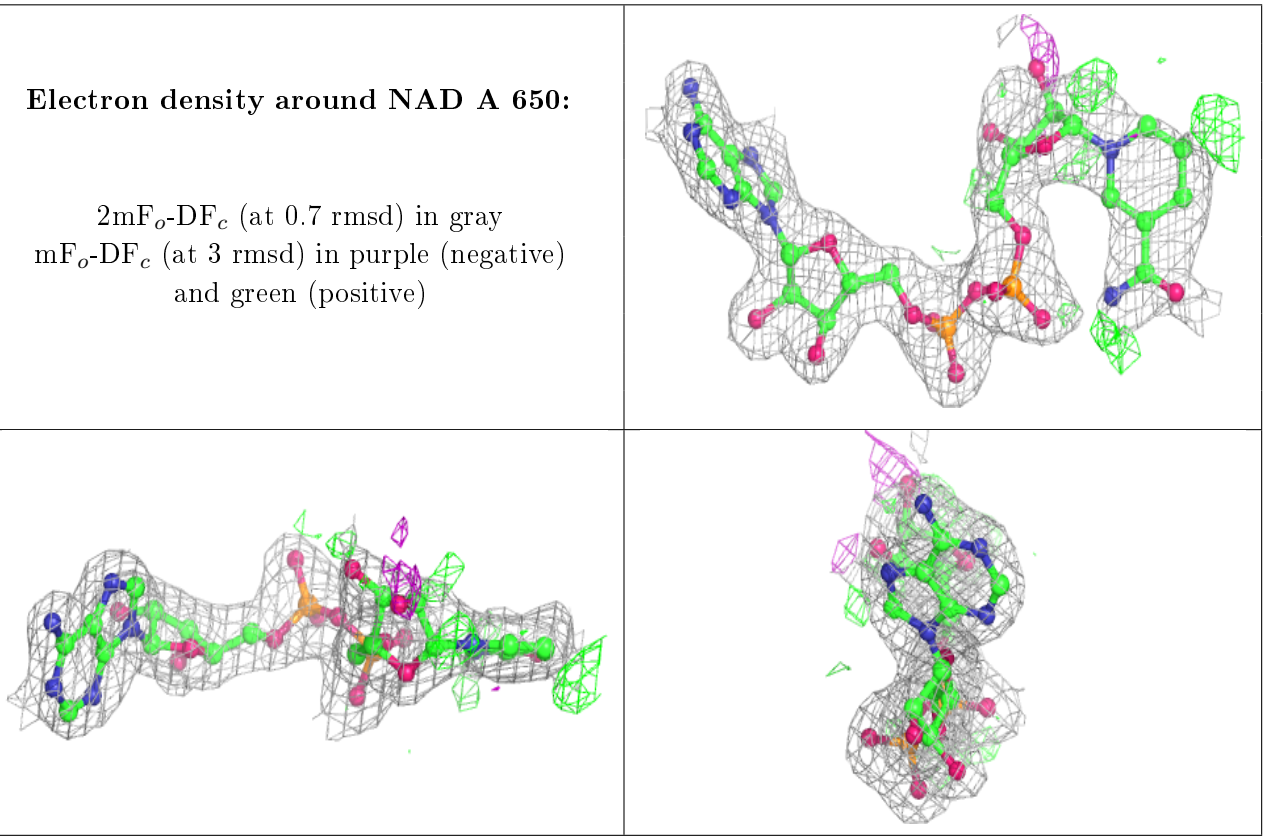
Electron density around NAD D 680:

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



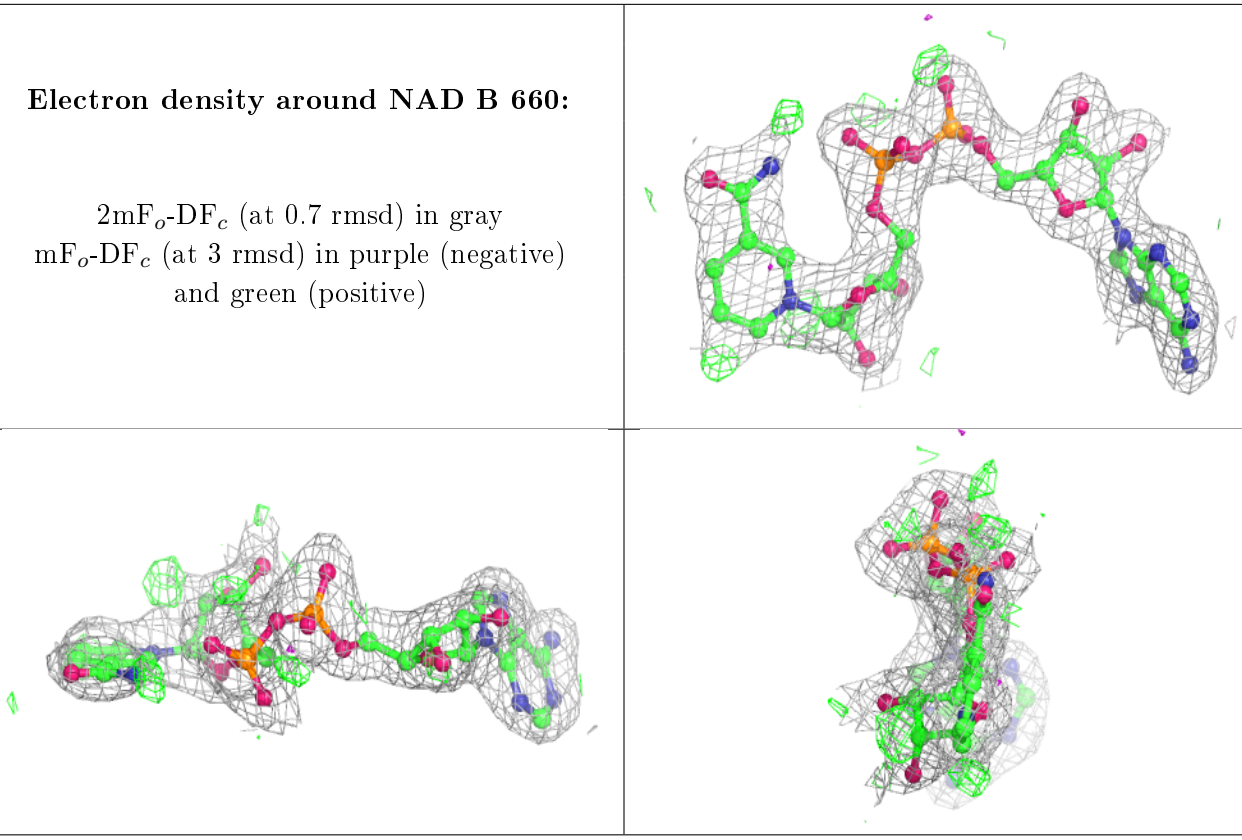
Electron density around NAD A 650:

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



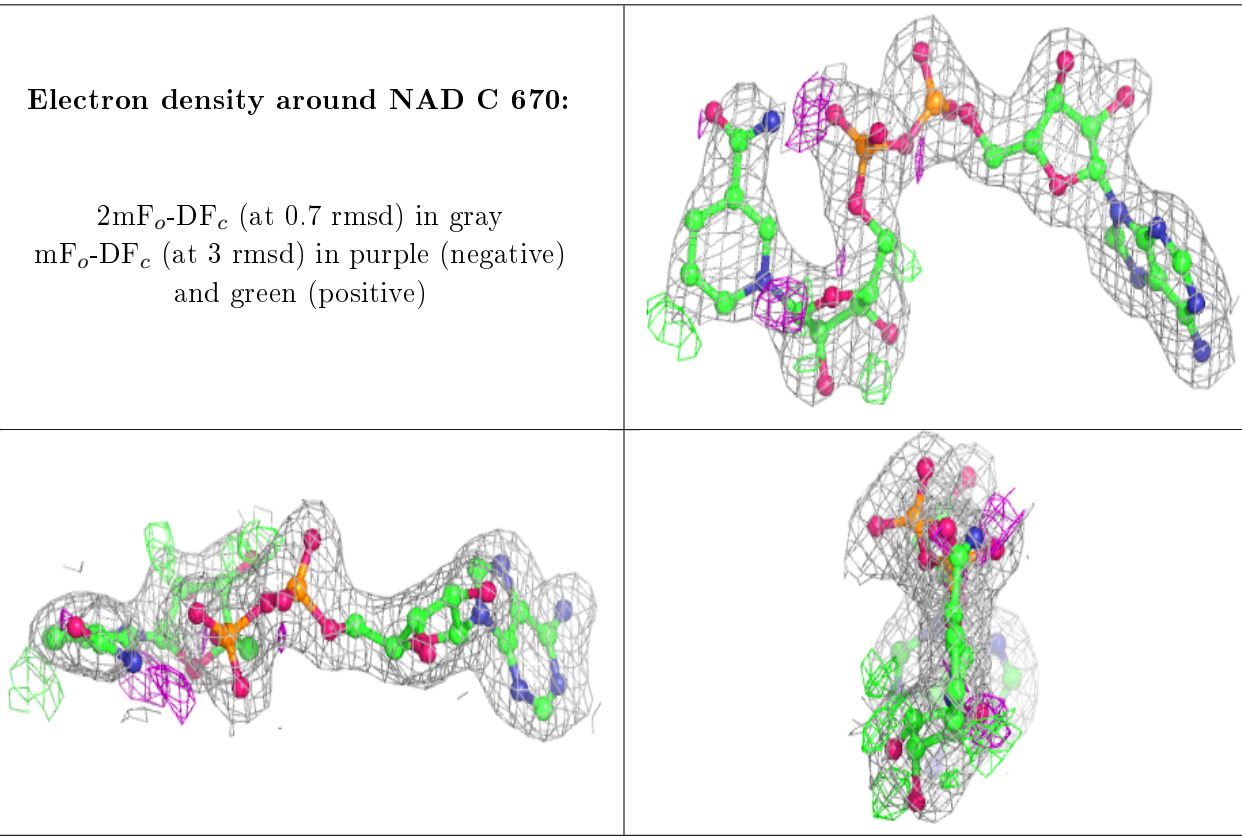
Electron density around NAD B 660:

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



Electron density around NAD C 670:

$2mF_o$-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.