Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:38 PM EDT

PDB ID	:	4A0M
Title	:	CRYSTAL STRUCTURE OF BETAINE ALDEHYDE DEHYDROGENASE FROM SPINACH IN COMPLEX WITH NAD
Authors	:	Gonzalez-Segura, L.; Rudino-Pinera, E.; Diaz-Sanchez, A.G.; Munoz-Clares, R.A.
Deposited on	:	2011-09-09
Resolution	:	2.30 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

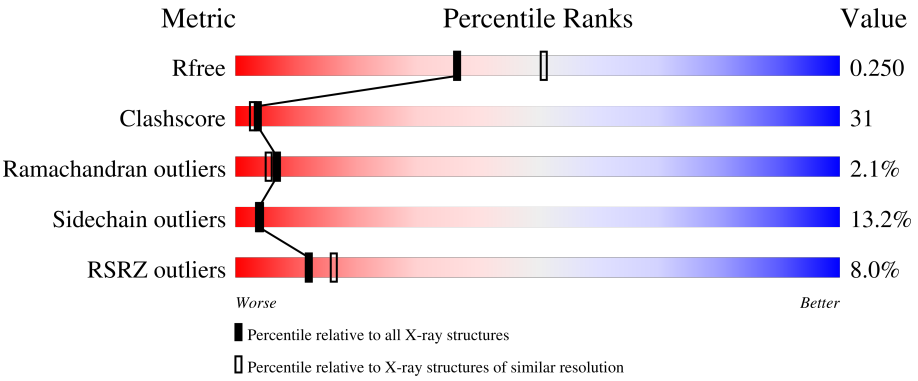
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	496	5% 54% 38% 8%
1	B	496	8% 54% 36% 9%
1	C	496	8% 53% 37% 9%
1	D	496	11% 51% 39% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	C	1499	-	-	X	-
4	GOL	D	1500	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16124 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.

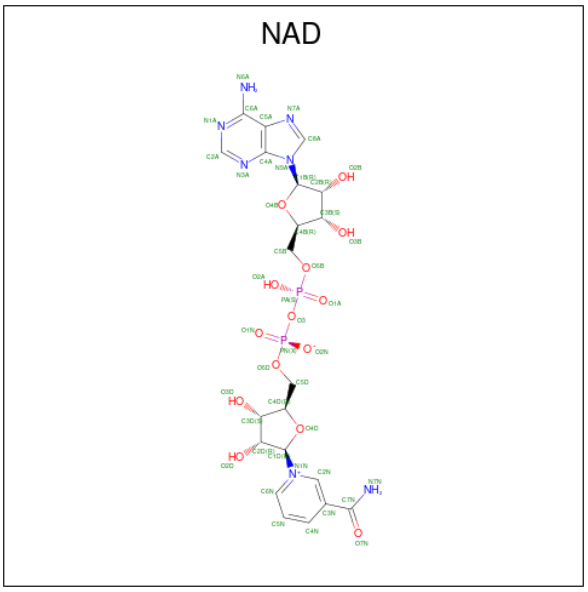
- Molecule 1 is a protein called BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	5	0
			3838	2461	637	723	17			
1	B	494	Total	C	N	O	S	0	6	0
			3844	2462	639	726	17			
1	C	494	Total	C	N	O	S	0	7	0
			3854	2471	640	726	17			
1	D	494	Total	C	N	O	S	0	5	0
			3838	2461	637	723	17			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

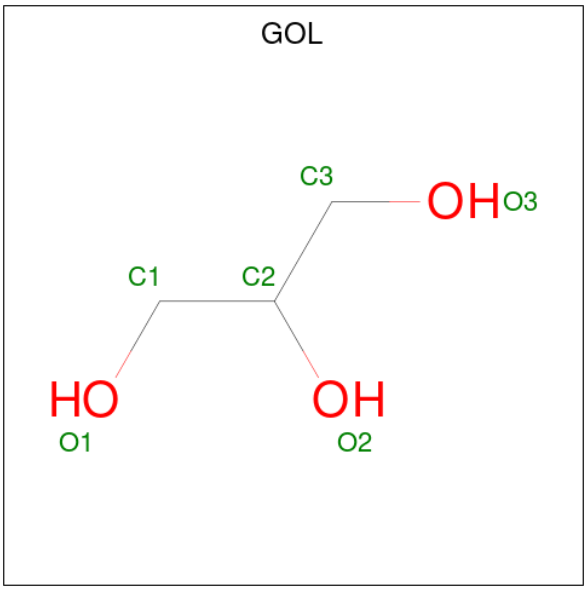
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	K	0	0
			2	2		
2	B	2	Total	K	0	0
			2	2		
2	C	3	Total	K	0	0
			3	3		
2	D	1	Total	K	0	0
			1	1		

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



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

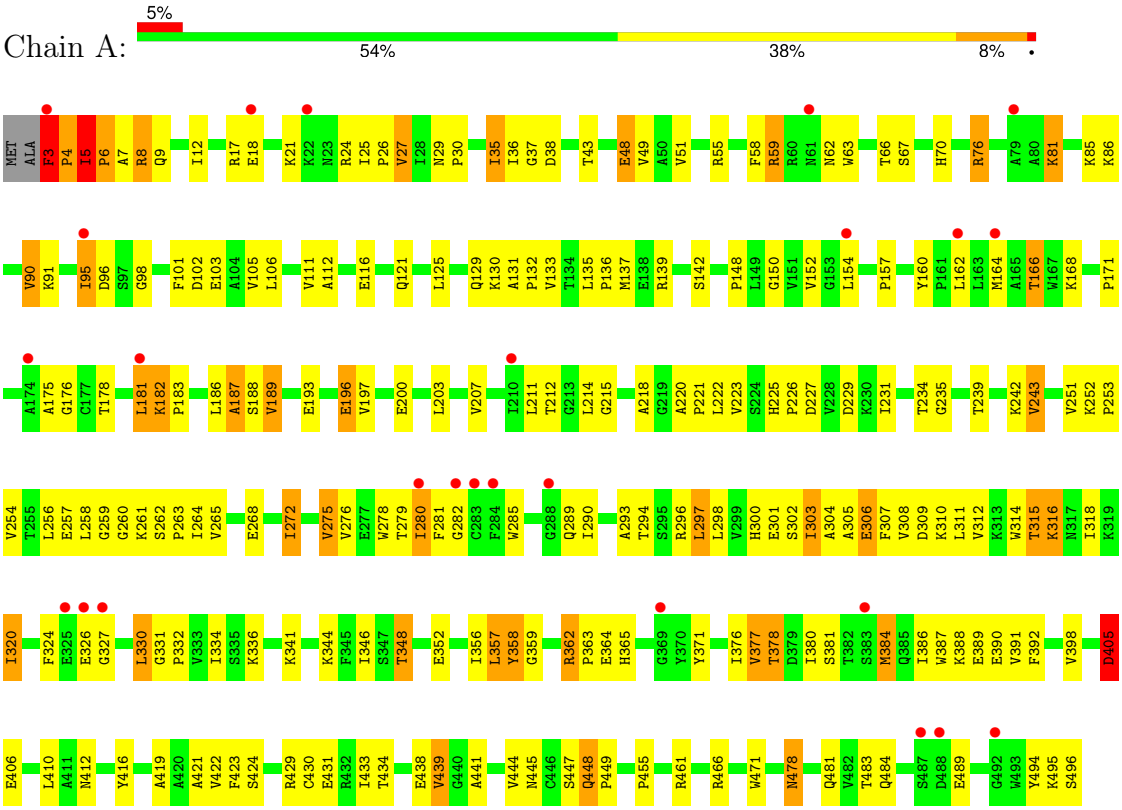
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	170	Total	O	0	0
			170	170		
5	B	128	Total	O	0	0
			128	128		
5	C	129	Total	O	0	0
			129	129		
5	D	97	Total	O	0	0
			97	97		

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.

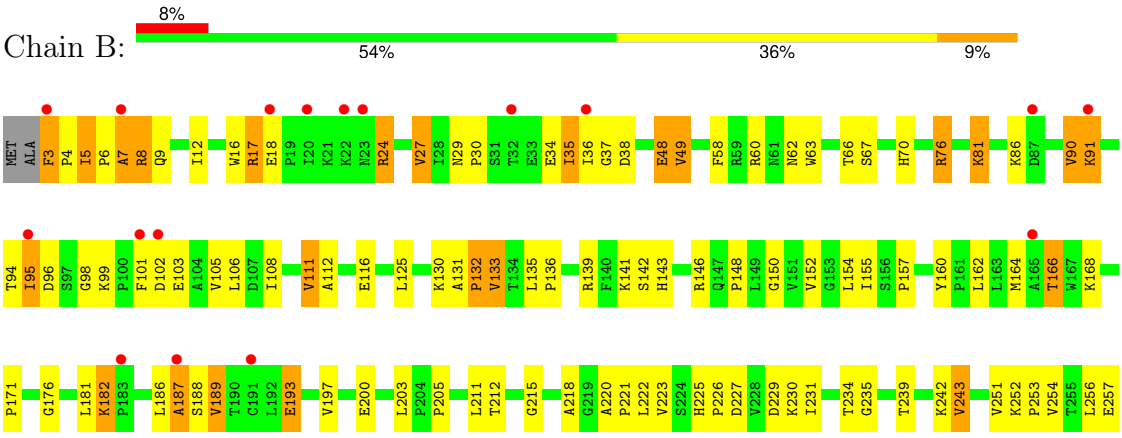
• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

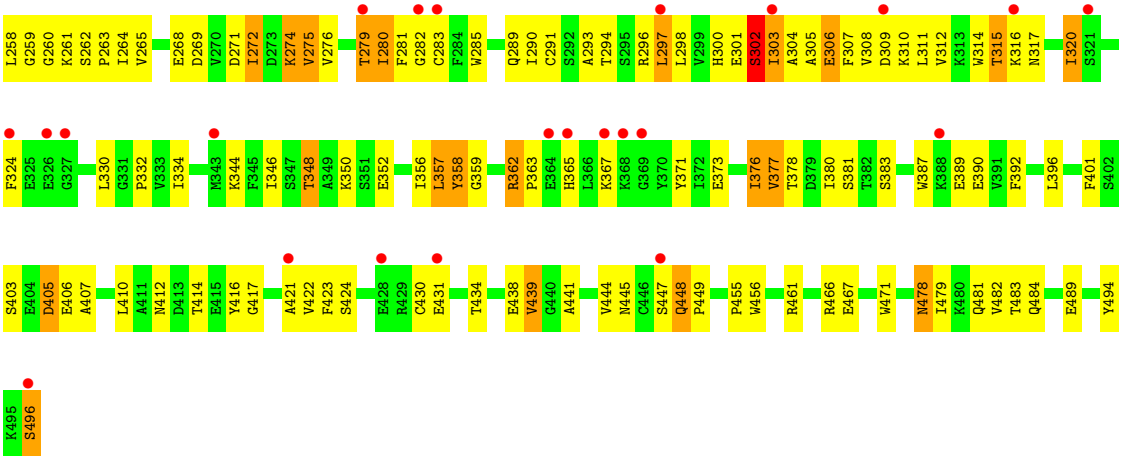
Chain A:



• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

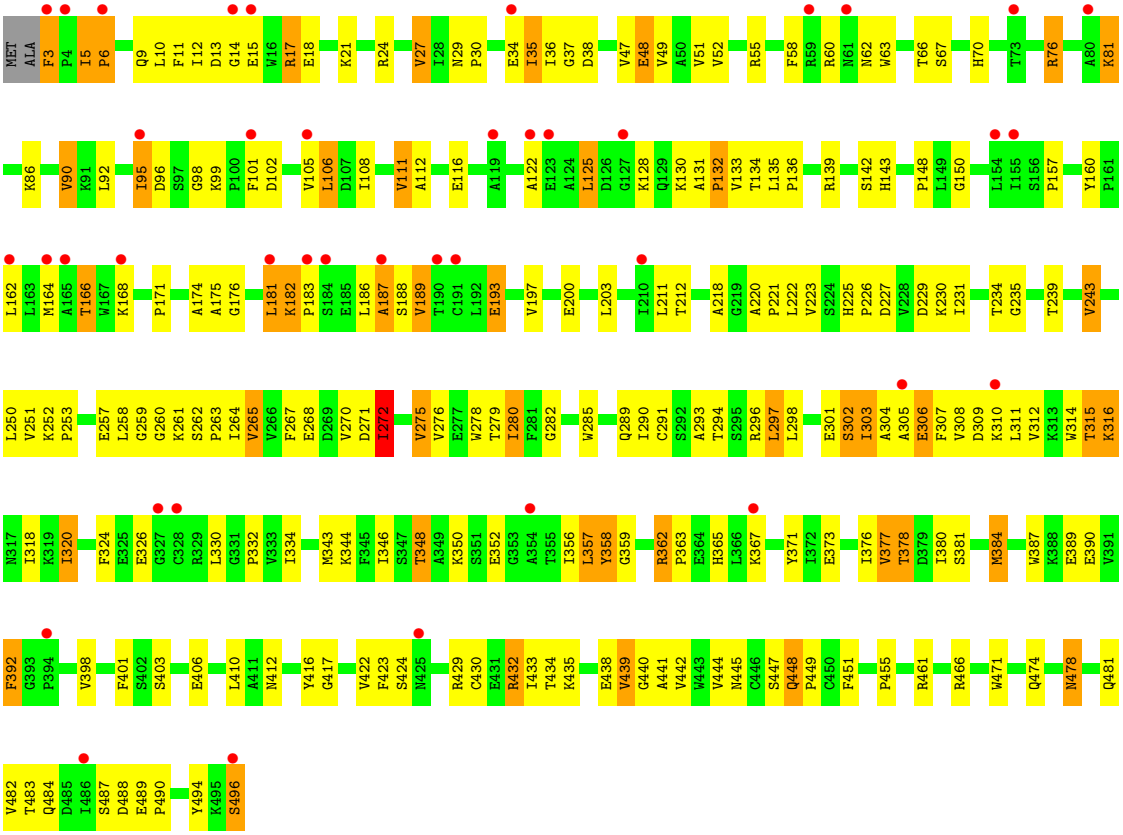
Chain B:





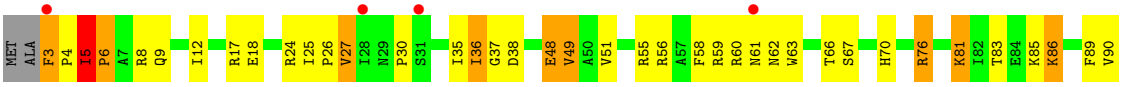
• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

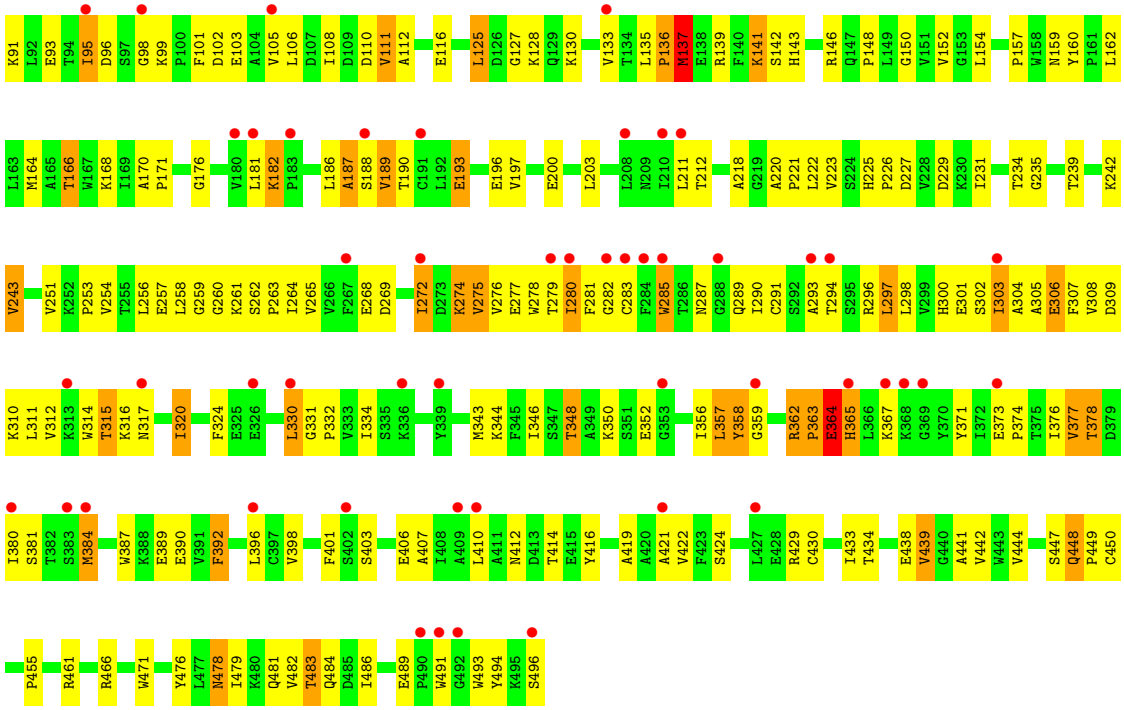
Chain C:



• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

Chain D:




K91 L92 E93 T94 I95 D96 S97 G98 K99 P100 F101 D102 E103 A104 V105 L106 D107 I108 D109 D110 V111 A112 E116 L125 D126 G127 K128 Q129 K130 V133 T134 L135 P136 M137 E138 R139 F140 K141 S142 H143 R146 Q147 P148 L149 G150 V151 V152 G153 L154 P157 W158 N159 Y160 P161 L162
L163 M164 A165 T166 W167 K168 I169 A170 P171 G176 V180 L181 K182 P183 L186 A187 S188 V189 T190 C191 L192 E193 E196 V197 E200 L203 L208 N209 I210 L211 T212 A218 G219 A220 P221 L222 V223 S224 H225 P226 D227 V228 D229 K230 I231 T234 G235 T239 K242
V243 V251 K252 P253 V254 T255 L256 E257 L258 G259 G260 K261 S262 P263 I264 V265 W266 F267 E268 D269 I272 D273 K274 V275 V276 E277 W278 T279 I280 F281 G282 C283 F284 W285 T286 N287 G288 Q289 I290 C291 S292 A293 T294 S295 R296 L297 L298 V299 H300 E301 S302 I303 A304 A305 E306 F307 V308 D309
K310 L311 V312 K313 W314 T315 K316 N317 I320 F324 E325 E326 L330 G331 P332 V333 I334 S335 K336 Y339 M343 K344 F345 I346 S347 T348 A349 K350 S351 E352 G353 I356 L357 Y358 G359 R362 P363 E364 H365 L366 K367 K368 G369 Y370 Y371 I372 E373 P374 T375 I376 V377 T378 D379
I380 S381 T382 S383 M384 W387 K388 E389 E390 V391 F392 L396 G397 V398 F401 S402 S403 E406 A407 I408 A409 L410 A411 N412 D413 T414 E415 Y416 A419 A420 A421 V422 F423 S424 L427 E428 R429 C430 I433 T434 E438 V439 G440 A441 V442 W443 V444 S447 Q448 P449 C450
P455 R461 R466 W471 Y476 L477 N478 I479 K480 Q481 V482 T483 Q484 D485 I486 E489 P490 W491 G492 W493 Y494 K495 S496

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.41Å 80.98Å 85.54Å 79.06° 84.94° 77.99°	Depositor
Resolution (Å)	29.08 – 2.30 29.08 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.6 (29.08-2.30) 90.2 (29.08-2.25)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.213 , 0.247 0.228 , 0.250	Depositor DCC
R_{free} test set	3811 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16124	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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, K, GOL

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	0.59	1/3932 (0.0%)	0.62	2/5349 (0.0%)
1	B	0.55	2/3938 (0.1%)	0.61	3/5356 (0.1%)
1	C	0.53	0/3948	0.59	0/5371
1	D	0.52	0/3932	0.60	0/5349
All	All	0.55	3/15750 (0.0%)	0.60	5/21425 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	ALA	C-N	-5.80	1.20	1.34
1	B	16	TRP	CB-CG	-5.48	1.40	1.50
1	A	278	TRP	CE3-CZ3	-5.17	1.29	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	7	ALA	O-C-N	7.04	133.96	122.70
1	B	7	ALA	C-N-CA	-6.12	106.41	121.70
1	A	405	ASP	CB-CG-OD1	-6.00	112.90	118.30
1	B	7	ALA	CA-C-N	-5.92	104.19	117.20
1	A	3	PHE	C-N-CD	-5.57	108.35	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	PHE	Peptide

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	3838	0	3831	237	0
1	B	3844	0	3829	241	0
1	C	3854	0	3846	266	0
1	D	3838	0	3831	281	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	26	5	0
3	B	44	0	26	9	0
3	C	44	0	26	8	0
3	D	44	0	26	6	0
4	A	12	0	16	1	0
4	C	6	0	8	8	0
4	D	24	0	32	9	0
5	A	170	0	0	13	0
5	B	128	0	0	14	0
5	C	129	0	0	10	0
5	D	97	0	0	10	0
All	All	16124	0	15497	974	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 31.

All (974) 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:60:ARG:CB	1:B:62[B]:ASN:HD21	1.14	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ARG:HB3	1:B:62[B]:ASN:ND2	1.17	1.46
1:A:6:PRO:HB2	1:A:7:ALA:CA	1.43	1.37
1:B:60:ARG:CB	1:B:62[B]:ASN:ND2	1.73	1.35
1:C:280:ILE:HG22	1:D:494:TYR:CE2	1.63	1.33
1:A:24:ARG:HD3	1:A:38:ASP:OD2	1.32	1.27
1:A:6:PRO:CB	1:A:7:ALA:HA	1.65	1.21
1:A:301:GLU:HB2	5:A:2094:HOH:O	1.38	1.18
1:C:55:ARG:HH12	4:C:1499:GOL:C3	1.57	1.17
1:D:450[B]:CYS:SG	4:D:1500:GOL:H2	1.87	1.14
1:A:5:ILE:HG22	1:A:6:PRO:N	1.64	1.11
1:C:270:VAL:HG21	1:C:275:VAL:HG11	1.29	1.11
1:C:270:VAL:CG2	1:C:275:VAL:HG11	1.84	1.06
1:C:280:ILE:CG2	1:D:494:TYR:CE2	2.38	1.06
1:B:5:ILE:HD11	1:B:95:ILE:HD11	1.36	1.03
1:D:450[B]:CYS:HG	4:D:1500:GOL:H2	1.05	1.03
1:D:3:PHE:CE2	1:D:95:ILE:HG21	1.95	1.01
1:A:76:ARG:HG3	1:A:76:ARG:HH11	1.25	0.99
1:B:24:ARG:HD3	1:B:38:ASP:OD2	1.63	0.99
1:A:6:PRO:HB2	1:A:7:ALA:CB	1.94	0.98
1:C:76:ARG:HH11	1:C:76:ARG:HG3	1.26	0.98
1:C:225:HIS:HD2	1:C:227:ASP:H	1.12	0.97
1:A:315:THR:HA	1:A:318:ILE:HD12	1.43	0.97
1:C:5:ILE:HG23	1:C:6:PRO:N	1.78	0.97
1:B:76:ARG:HG3	1:B:76:ARG:HH11	1.29	0.97
1:D:225:HIS:HD2	1:D:227:ASP:H	1.11	0.97
1:D:297:LEU:HB2	5:D:2071:HOH:O	1.64	0.97
1:D:320:ILE:HG21	1:D:373:GLU:OE2	1.65	0.96
1:B:271:ASP:CG	1:B:274:LYS:HD2	1.85	0.95
1:C:5:ILE:CG2	1:C:6:PRO:N	2.30	0.95
1:C:96:ASP:OD2	1:C:189:VAL:HG13	1.66	0.95
1:A:6:PRO:CB	1:A:7:ALA:CA	2.30	0.94
1:A:3:PHE:CD1	1:A:3:PHE:N	2.32	0.94
1:D:76:ARG:HG3	1:D:76:ARG:HH11	1.29	0.94
1:A:6:PRO:HB2	1:A:7:ALA:HA	0.94	0.93
1:D:110:ASP:OD2	4:D:1501:GOL:H2	1.65	0.93
1:B:60:ARG:HB2	1:B:62[B]:ASN:HD21	0.78	0.92
1:C:24:ARG:HD3	1:C:38:ASP:OD2	1.69	0.92
1:C:280:ILE:HG22	1:D:494:TYR:HE2	1.01	0.91
1:A:225:HIS:HD2	1:A:227:ASP:H	1.14	0.91
1:A:3:PHE:N	1:A:3:PHE:HD1	1.70	0.90
1:B:225:HIS:HD2	1:B:227:ASP:H	1.13	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:PHE:N	1:B:4:PRO:HD2	1.88	0.89
1:C:5:ILE:HG23	1:C:6:PRO:CD	2.01	0.89
1:C:55:ARG:NH1	4:C:1499:GOL:C3	2.36	0.87
1:C:316:LYS:HD2	1:C:358:TYR:HE2	1.39	0.87
1:D:95:ILE:HG22	1:D:324:PHE:CZ	2.09	0.86
1:D:363:PRO:O	1:D:364:GLU:HB2	1.73	0.86
1:D:5:ILE:HD13	1:D:5:ILE:H	1.41	0.85
1:A:242:LYS:HE2	1:D:127:GLY:CA	2.07	0.85
1:B:268:GLU:HA	1:B:303:ILE:HD11	1.57	0.85
1:B:60:ARG:HB3	1:B:62[B]:ASN:HD22	1.07	0.85
1:C:225:HIS:CD2	1:C:227:ASP:H	1.95	0.85
1:D:225:HIS:CD2	1:D:227:ASP:H	1.95	0.84
1:C:15:GLU:HG2	1:C:17:ARG:HH11	1.43	0.83
1:C:272:ILE:HG13	1:C:272:ILE:O	1.78	0.83
1:C:150:GLY:HA3	4:C:1499:GOL:O3	1.76	0.83
1:D:268:GLU:HA	1:D:303:ILE:HD11	1.58	0.83
1:B:3:PHE:HB2	1:B:91:LYS:HZ1	1.43	0.82
1:B:225:HIS:CD2	1:B:227:ASP:H	1.97	0.82
1:C:102:ASP:O	1:C:105:VAL:HG22	1.80	0.82
1:B:5:ILE:HD11	1:B:95:ILE:CD1	2.08	0.82
1:D:24:ARG:HD3	1:D:38:ASP:OD2	1.79	0.82
1:A:225:HIS:CD2	1:A:227:ASP:H	1.97	0.82
1:C:55:ARG:HH12	4:C:1499:GOL:H31	1.44	0.82
1:D:5:ILE:H	1:D:5:ILE:CD1	1.93	0.82
1:D:272:ILE:HD12	1:D:307:PHE:HA	1.60	0.82
1:A:5:ILE:CG2	1:A:6:PRO:N	2.39	0.81
1:A:481:GLN:HE21	1:A:483:THR:HG21	1.44	0.81
1:C:305:ALA:O	1:C:306:GLU:HB3	1.80	0.81
1:A:341:LYS:HE3	5:A:2110:HOH:O	1.79	0.81
1:C:268:GLU:HA	1:C:303:ILE:HD11	1.62	0.81
1:A:272:ILE:HD12	1:A:307:PHE:HA	1.61	0.81
1:D:95:ILE:HG22	1:D:324:PHE:HZ	1.46	0.81
1:A:481:GLN:HE21	1:A:483:THR:CG2	1.93	0.81
1:D:481:GLN:HE21	1:D:483:THR:HG21	1.46	0.81
1:B:272:ILE:HD12	1:B:307:PHE:HA	1.62	0.80
1:B:481:GLN:HE21	1:B:483:THR:CG2	1.94	0.80
1:D:3:PHE:CZ	1:D:95:ILE:HG21	2.16	0.80
1:C:101:PHE:O	1:C:105:VAL:HG13	1.82	0.79
1:C:481:GLN:HE21	1:C:483:THR:CG2	1.95	0.79
1:A:162:LEU:O	1:A:166:THR:HG23	1.83	0.79
1:D:157:PRO:HG3	1:D:234:THR:HG22	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:HG23	1:C:6:PRO:HD2	1.65	0.79
1:A:268:GLU:HA	1:A:303:ILE:HD11	1.66	0.78
1:B:95:ILE:HG22	1:B:324:PHE:CE2	2.17	0.78
1:A:24:ARG:CD	1:A:38:ASP:OD2	2.23	0.78
1:C:5:ILE:HD11	1:C:95:ILE:HD11	1.63	0.78
1:D:481:GLN:HE21	1:D:483:THR:CG2	1.95	0.78
1:C:142:SER:OG	1:C:483:THR:HG22	1.84	0.78
1:A:95:ILE:HG22	1:A:324:PHE:CE2	2.17	0.77
1:C:481:GLN:HE21	1:C:483:THR:HG21	1.47	0.77
1:D:55:ARG:O	1:D:59:ARG:HG3	1.84	0.77
1:B:162:LEU:O	1:B:166:THR:HG23	1.84	0.77
1:A:5:ILE:H	1:A:6:PRO:HD3	1.50	0.77
1:C:9:GLN:OE1	1:C:18:GLU:HA	1.84	0.77
1:A:51:VAL:HG21	1:A:225:HIS:CE1	2.20	0.76
1:A:344:LYS:O	1:A:348:THR:HG23	1.86	0.76
1:C:162:LEU:O	1:C:166:THR:HG23	1.84	0.76
1:A:9:GLN:OE1	1:A:18:GLU:HA	1.85	0.76
1:A:242:LYS:HE2	1:D:127:GLY:HA2	1.65	0.76
1:D:320:ILE:HD11	1:D:371:TYR:CD1	2.21	0.76
1:A:362:ARG:HD3	1:A:363:PRO:HD2	1.66	0.76
1:D:51:VAL:HG21	1:D:225:HIS:CE1	2.21	0.76
1:B:9:GLN:OE1	1:B:18:GLU:HA	1.86	0.76
1:B:3:PHE:N	1:B:4:PRO:CD	2.49	0.76
1:B:95:ILE:HG22	1:B:324:PHE:CZ	2.21	0.75
1:B:261:LYS:HG3	1:B:296:ARG:HD2	1.68	0.75
1:D:365:HIS:H	1:D:365:HIS:CD2	2.03	0.75
1:A:455:PRO:HG3	1:A:471:TRP:CZ3	2.21	0.75
1:B:390[B]:GLU:OE2	5:B:2102:HOH:O	2.04	0.75
1:D:9:GLN:OE1	1:D:18:GLU:HA	1.87	0.75
1:B:320:ILE:HD11	1:B:371:TYR:CD1	2.22	0.75
1:D:260:GLY:HA2	1:D:416:TYR:CD1	2.22	0.75
1:D:278:TRP:O	1:D:281:PHE:N	2.20	0.75
1:C:5:ILE:HD11	1:C:95:ILE:CD1	2.17	0.75
1:C:362:ARG:HD3	1:C:363:PRO:HD2	1.68	0.75
1:C:429:ARG:HA	1:C:432:ARG:NH2	2.02	0.75
1:B:362:ARG:HD3	1:B:363:PRO:HD2	1.69	0.75
1:B:5:ILE:HG22	1:B:6:PRO:O	1.86	0.74
1:C:95:ILE:HG22	1:C:324:PHE:CE2	2.21	0.74
1:A:142:SER:OG	1:A:483:THR:HG22	1.87	0.74
1:D:320:ILE:HD11	1:D:371:TYR:HD1	1.51	0.74
1:B:275:VAL:O	1:B:279:THR:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:PHE:CB	1:B:91:LYS:HZ1	2.01	0.74
1:C:15:GLU:CG	1:C:17:ARG:HH11	2.01	0.74
1:C:267:PHE:O	1:C:270:VAL:CG1	2.35	0.74
1:D:162:LEU:O	1:D:166:THR:HG23	1.86	0.73
1:B:142:SER:OG	1:B:483:THR:HG22	1.88	0.73
1:C:455:PRO:HG3	1:C:471:TRP:CZ3	2.23	0.73
1:D:3:PHE:CG	1:D:91:LYS:NZ	2.56	0.73
1:B:320:ILE:HD11	1:B:371:TYR:HD1	1.53	0.73
1:C:270:VAL:CG2	1:C:275:VAL:CG1	2.66	0.73
1:C:316:LYS:HD2	1:C:358:TYR:CE2	2.23	0.73
1:D:297:LEU:N	5:D:2071:HOH:O	2.21	0.73
1:B:60:ARG:HB2	1:B:62[B]:ASN:ND2	1.64	0.73
1:C:261:LYS:HG3	1:C:296:ARG:HD2	1.70	0.73
1:C:430:CYS:O	1:C:434:THR:HG23	1.89	0.73
1:A:280:ILE:HG22	1:B:494:TYR:CE2	2.23	0.72
1:A:289:GLN:HE22	1:A:334:ILE:H	1.37	0.72
1:B:157:PRO:HG3	1:B:234:THR:HG22	1.69	0.72
1:A:96:ASP:OD2	1:A:189:VAL:HG13	1.89	0.72
1:A:130:LYS:NZ	1:B:431:GLU:OE1	2.22	0.72
1:A:157:PRO:HG3	1:A:234:THR:HG22	1.72	0.72
1:B:481:GLN:HE21	1:B:483:THR:HG21	1.53	0.72
1:D:3:PHE:HE2	1:D:95:ILE:HG21	1.50	0.72
1:D:430:CYS:O	1:D:434:THR:HG23	1.89	0.72
1:A:261:LYS:HG3	1:A:296:ARG:HD2	1.70	0.72
1:C:320:ILE:HD11	1:C:371:TYR:CD1	2.24	0.72
1:D:396:LEU:HD21	5:D:2071:HOH:O	1.88	0.72
1:A:95:ILE:HG22	1:A:324:PHE:CZ	2.25	0.72
1:D:274:LYS:O	1:D:277:GLU:N	2.23	0.72
1:D:311:LEU:O	1:D:315:THR:HG22	1.90	0.71
1:C:135:LEU:HD21	1:C:142:SER:CB	2.21	0.71
1:D:289:GLN:HE22	1:D:334:ILE:H	1.39	0.71
1:B:300:HIS:ND1	1:B:302:SER:HB2	2.05	0.71
1:C:251[A]:VAL:HG11	1:D:258:LEU:HD11	1.72	0.71
1:B:430:CYS:O	1:B:434:THR:HG23	1.90	0.71
1:D:5:ILE:CD1	1:D:5:ILE:N	2.53	0.71
1:D:455:PRO:HG3	1:D:471:TRP:CZ3	2.25	0.71
1:B:455:PRO:HG3	1:B:471:TRP:CZ3	2.26	0.71
1:A:135:LEU:HD21	1:A:142:SER:CB	2.21	0.71
1:A:260:GLY:HA2	1:A:416:TYR:CD1	2.25	0.71
1:A:320:ILE:HD11	1:A:371:TYR:CD1	2.26	0.71
1:B:357:LEU:HD23	1:B:357:LEU:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251[A]:VAL:HG12	1:C:251[A]:VAL:O	1.91	0.70
1:C:157:PRO:HG3	1:C:234:THR:HG22	1.73	0.70
1:D:344:LYS:O	1:D:348:THR:HG23	1.91	0.70
1:A:430:CYS:O	1:A:434:THR:HG23	1.91	0.70
1:B:260:GLY:HA2	1:B:416:TYR:CD1	2.26	0.70
1:B:271:ASP:CG	1:B:274:LYS:CD	2.59	0.70
1:C:320:ILE:HD11	1:C:371:TYR:HD1	1.56	0.70
1:D:414:THR:CG2	5:D:2070:HOH:O	2.40	0.70
1:C:272:ILE:O	1:C:272:ILE:CG1	2.39	0.70
1:D:5:ILE:HG12	1:D:36:ILE:HG13	1.74	0.70
1:B:135:LEU:HD21	1:B:142:SER:CB	2.22	0.70
1:B:261:LYS:HG3	1:B:296:ARG:CD	2.21	0.70
1:C:344:LYS:O	1:C:348:THR:HG23	1.92	0.70
1:C:270:VAL:HG23	1:C:275:VAL:HG11	1.74	0.70
1:D:261:LYS:HG3	1:D:296:ARG:HD2	1.73	0.70
1:A:251:VAL:HG11	1:B:258:LEU:HD11	1.73	0.70
1:C:260:GLY:HA2	1:C:416:TYR:CD1	2.26	0.69
1:D:450[B]:CYS:SG	4:D:1500:GOL:C2	2.76	0.69
1:D:63:TRP:O	1:D:66:THR:HB	1.92	0.69
1:D:275:VAL:O	1:D:279:THR:HG23	1.92	0.69
1:D:261:LYS:HG3	1:D:296:ARG:CD	2.23	0.69
1:D:112:ALA:O	1:D:116:GLU:HG3	1.93	0.69
1:D:135:LEU:HD21	1:D:142:SER:CB	2.23	0.69
1:D:272:ILE:HA	1:D:275:VAL:HG13	1.75	0.69
1:B:63:TRP:O	1:B:66:THR:HB	1.91	0.69
1:D:142:SER:OG	1:D:483:THR:HG22	1.92	0.69
1:B:289:GLN:HE22	1:B:334:ILE:H	1.41	0.69
1:B:414:THR:HG22	5:B:2108:HOH:O	1.92	0.69
1:C:55:ARG:HH12	4:C:1499:GOL:H32	1.55	0.69
1:C:76:ARG:HG3	1:C:76:ARG:NH1	2.05	0.69
1:C:95:ILE:HG22	1:C:324:PHE:CZ	2.27	0.69
1:C:272:ILE:HA	1:C:275:VAL:HG13	1.75	0.69
1:C:289:GLN:HE22	1:C:334:ILE:H	1.38	0.69
1:C:482:VAL:HG21	5:C:2039:HOH:O	1.93	0.69
1:A:63:TRP:O	1:A:66:THR:HB	1.93	0.69
1:B:311:LEU:O	1:B:315:THR:HG22	1.92	0.69
1:C:311:LEU:O	1:C:315:THR:HG22	1.93	0.69
1:A:261:LYS:HG3	1:A:296:ARG:CD	2.22	0.69
1:A:357:LEU:O	1:A:357:LEU:HD23	1.93	0.69
1:A:275:VAL:O	1:A:279:THR:HG23	1.93	0.68
1:C:357:LEU:HD23	1:C:357:LEU:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:LEU:O	1:D:357:LEU:HD23	1.93	0.68
1:B:242:LYS:NZ	5:B:2080:HOH:O	2.25	0.68
1:C:435:LYS:HE2	5:C:2103:HOH:O	1.93	0.68
1:D:3:PHE:HE2	1:D:95:ILE:HD12	1.59	0.68
1:B:3:PHE:HB2	1:B:91:LYS:NZ	2.09	0.68
1:C:76:ARG:HH11	1:C:76:ARG:CG	2.06	0.68
1:D:196:GLU:HG2	5:D:2002:HOH:O	1.93	0.68
1:D:3:PHE:HZ	1:D:324:PHE:CZ	2.12	0.68
1:D:182:LYS:HD2	1:D:218:ALA:HB3	1.76	0.68
1:B:96:ASP:OD2	1:B:189:VAL:HG13	1.94	0.67
1:B:272:ILE:HA	1:B:275:VAL:HG13	1.75	0.67
1:C:267:PHE:O	1:C:270:VAL:HG13	1.94	0.67
1:C:96:ASP:OD2	1:C:189:VAL:CG1	2.40	0.67
1:C:258:LEU:HD11	1:D:251:VAL:HG11	1.75	0.67
1:C:275:VAL:O	1:C:279:THR:HG23	1.95	0.67
1:A:76:ARG:HH11	1:A:76:ARG:CG	2.03	0.67
1:C:270:VAL:HG23	1:C:275:VAL:CG1	2.25	0.67
1:A:215:GLY:HA3	3:A:1498:NAD:C8A	2.24	0.67
1:A:444:VAL:HB	1:B:484:GLN:CB	2.25	0.67
1:D:305:ALA:O	1:D:306:GLU:CB	2.43	0.67
1:B:5:ILE:CG2	1:B:6:PRO:O	2.43	0.67
1:A:251:VAL:O	1:A:251:VAL:HG12	1.95	0.67
1:A:258:LEU:HD11	1:B:251:VAL:HG11	1.76	0.66
1:C:305:ALA:O	1:C:306:GLU:CB	2.43	0.66
1:D:9:GLN:NE2	1:D:24:ARG:HH21	1.93	0.66
1:A:320:ILE:HD11	1:A:371:TYR:HD1	1.57	0.66
1:A:272:ILE:HA	1:A:275:VAL:HG13	1.77	0.66
1:A:431:GLU:HB2	5:A:2136:HOH:O	1.95	0.66
1:B:76:ARG:HH11	1:B:76:ARG:CG	2.06	0.66
1:D:390[B]:GLU:O	1:D:390[B]:GLU:HG3	1.94	0.66
1:A:81:LYS:HD3	1:A:200:GLU:OE1	1.96	0.66
1:B:406:GLU:O	1:B:410:LEU:HB2	1.96	0.66
1:D:4:PRO:C	1:D:5:ILE:O	2.30	0.66
1:A:259:GLY:HA3	3:A:1498:NAD:O2D	1.96	0.66
1:B:3:PHE:CB	1:B:91:LYS:NZ	2.59	0.66
1:D:135:LEU:HD21	1:D:142:SER:HB3	1.77	0.66
1:B:6:PRO:HG2	1:B:193:GLU:OE2	1.96	0.65
1:B:357:LEU:O	1:B:358:TYR:HB2	1.96	0.65
1:C:63:TRP:O	1:C:66:THR:HB	1.97	0.65
1:D:493:TRP:HD1	1:D:494:TYR:CE1	2.14	0.65
1:C:55:ARG:NH1	4:C:1499:GOL:H32	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLU:HG2	1:A:310:LYS:HZ3	1.61	0.65
1:D:272:ILE:HD13	1:D:306:GLU:HG2	1.77	0.65
1:C:390[B]:GLU:HG3	1:C:390[B]:GLU:O	1.97	0.65
1:B:6:PRO:CG	1:B:193:GLU:OE2	2.45	0.65
1:B:251:VAL:HG12	1:B:251:VAL:O	1.96	0.65
1:C:261:LYS:HG3	1:C:296:ARG:CD	2.26	0.65
1:D:272:ILE:CD1	1:D:306:GLU:HG2	2.27	0.65
1:C:306:GLU:O	1:C:310:LYS:HG2	1.96	0.65
1:B:390[B]:GLU:O	1:B:390[B]:GLU:HG3	1.97	0.65
1:D:3:PHE:HZ	1:D:324:PHE:HZ	1.44	0.65
1:A:405:ASP:OD1	1:A:405:ASP:C	2.30	0.64
1:C:272:ILE:HD11	1:C:306:GLU:HG2	1.78	0.64
1:D:314:TRP:O	1:D:317:ASN:HB2	1.97	0.64
1:B:168:LYS:O	1:B:171:PRO:HD2	1.98	0.64
1:B:271:ASP:OD2	1:B:274:LYS:NZ	2.29	0.64
1:C:259:GLY:H	3:C:1498:NAD:H71N	1.45	0.64
1:C:365:HIS:CD2	1:C:365:HIS:H	2.13	0.64
1:A:66:THR:HG22	1:A:67:SER:O	1.98	0.64
1:D:3:PHE:CZ	1:D:95:ILE:CG2	2.80	0.64
1:D:259:GLY:HA3	3:D:1498:NAD:O2D	1.98	0.64
1:A:5:ILE:HG22	1:A:6:PRO:CA	2.28	0.64
1:D:76:ARG:HH11	1:D:76:ARG:CG	2.09	0.64
1:D:274:LYS:O	1:D:275:VAL:C	2.35	0.64
1:A:30:PRO:HB2	1:A:332:PRO:HG2	1.79	0.64
1:B:365:HIS:H	1:B:365:HIS:CD2	2.15	0.64
1:C:251[A]:VAL:HG11	1:D:258:LEU:CD1	2.28	0.64
1:A:305:ALA:O	1:A:306:GLU:HB2	1.99	0.63
1:C:34:GLU:O	1:C:36:ILE:HG23	1.98	0.63
5:A:2162:HOH:O	1:B:314:TRP:HE3	1.81	0.63
1:B:182:LYS:HD2	1:B:218:ALA:HB3	1.79	0.63
1:A:251:VAL:HG11	1:B:258:LEU:CD1	2.29	0.63
1:C:66:THR:HG22	1:C:67:SER:O	1.99	0.63
1:A:390[B]:GLU:O	1:A:390[B]:GLU:HG3	1.97	0.63
1:B:308:VAL:O	1:B:312:VAL:HG13	1.99	0.63
1:C:182:LYS:HD2	1:C:218:ALA:HB3	1.80	0.63
1:A:76:ARG:HG3	1:A:76:ARG:NH1	2.04	0.62
1:B:447:SER:C	1:B:449:PRO:HD3	2.20	0.62
1:C:6:PRO:HB3	1:C:193:GLU:OE2	1.98	0.62
1:D:396:LEU:CD2	5:D:2071:HOH:O	2.46	0.62
1:C:455:PRO:HG3	1:C:471:TRP:CE3	2.34	0.62
1:C:3:PHE:CD1	1:C:3:PHE:C	2.67	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LEU:HD21	1:B:387:TRP:HH2	1.65	0.62
1:C:135:LEU:HD21	1:C:142:SER:HB2	1.81	0.62
1:C:377:VAL:CG2	1:C:380:ILE:HD11	2.29	0.62
1:D:291:CYS:HB3	3:D:1498:NAD:C6N	2.29	0.62
1:A:306:GLU:HG2	1:A:310:LYS:NZ	2.13	0.62
1:A:494:TYR:HB3	5:A:2162:HOH:O	2.00	0.62
1:B:103:GLU:OE2	1:B:285:TRP:CD1	2.53	0.62
1:B:412:ASN:HD21	1:B:438:GLU:H	1.48	0.61
1:C:12:ILE:HD11	1:C:211:LEU:HD21	1.81	0.61
1:C:259:GLY:HA3	3:C:1498:NAD:O2D	1.99	0.61
1:D:76:ARG:HG3	1:D:76:ARG:NH1	2.07	0.61
1:D:251:VAL:HG12	1:D:251:VAL:O	1.99	0.61
1:C:9:GLN:NE2	1:C:24:ARG:HH21	1.97	0.61
1:D:312:VAL:O	1:D:316:LYS:HB2	2.01	0.61
1:A:305:ALA:O	1:A:306:GLU:CB	2.49	0.61
1:C:298:LEU:HD21	1:C:387:TRP:HH2	1.65	0.61
1:C:312:VAL:O	1:C:316:LYS:HB2	2.00	0.61
1:C:412:ASN:HD21	1:C:438:GLU:H	1.49	0.61
1:D:493:TRP:CD1	1:D:494:TYR:CE1	2.88	0.61
1:B:350:LYS:HE3	1:B:356:ILE:HD12	1.81	0.61
1:C:447:SER:C	1:C:449:PRO:HD3	2.21	0.61
1:A:377:VAL:CG2	1:A:380:ILE:HD11	2.31	0.61
1:A:298:LEU:HD21	1:A:387:TRP:HH2	1.66	0.61
3:C:1498:NAD:H52A	3:C:1498:NAD:O2N	2.01	0.61
1:A:455:PRO:HG3	1:A:471:TRP:CE3	2.36	0.60
1:C:258:LEU:CD1	1:D:251:VAL:HG11	2.31	0.60
1:C:444:VAL:HB	1:D:484:GLN:CB	2.31	0.60
1:C:105:VAL:HG23	1:C:106:LEU:HD13	1.83	0.60
1:A:135:LEU:HD21	1:A:142:SER:HB3	1.82	0.60
1:B:17:ARG:HG2	5:B:2006:HOH:O	2.01	0.60
1:B:76:ARG:HG3	1:B:76:ARG:NH1	2.09	0.60
1:D:66:THR:CG2	1:D:70:HIS:HB3	2.31	0.60
1:A:494:TYR:CE2	1:B:280:ILE:HG22	2.36	0.60
1:C:66:THR:CG2	1:C:70:HIS:HB3	2.31	0.60
1:D:265:VAL:HG22	1:D:422:VAL:HG23	1.84	0.60
1:A:168:LYS:O	1:A:171:PRO:HD2	2.02	0.60
1:D:3:PHE:CE2	1:D:95:ILE:CG2	2.80	0.60
1:B:265:VAL:HG22	1:B:422:VAL:HG23	1.83	0.60
1:D:3:PHE:CB	1:D:91:LYS:NZ	2.64	0.60
1:C:150:GLY:CA	4:C:1499:GOL:O3	2.48	0.60
1:D:298:LEU:HD21	1:D:387:TRP:HH2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:O	1:A:315:THR:HG22	2.02	0.59
1:D:27:VAL:HG13	1:D:37:GLY:C	2.23	0.59
1:C:377:VAL:HG22	1:C:380:ILE:HD11	1.84	0.59
1:C:81:LYS:HG2	1:C:197:VAL:HG13	1.84	0.59
1:D:412:ASN:HD21	1:D:438:GLU:H	1.49	0.59
1:A:316:LYS:HD2	1:A:358:TYR:HE2	1.67	0.59
1:B:377:VAL:CG2	1:B:380:ILE:HD11	2.33	0.59
1:A:6:PRO:HB2	1:A:7:ALA:HB2	1.82	0.59
1:B:66:THR:CG2	1:B:70:HIS:HB3	2.32	0.59
1:B:81:LYS:HG2	1:B:197:VAL:HG13	1.85	0.59
1:C:135:LEU:HD21	1:C:142:SER:HB3	1.85	0.59
1:C:315:THR:HG23	5:C:2074:HOH:O	2.01	0.59
1:D:377:VAL:CG2	1:D:380:ILE:HD11	2.32	0.59
1:A:135:LEU:HD21	1:A:142:SER:HB2	1.84	0.59
1:B:377:VAL:HG22	1:B:380:ILE:HD11	1.84	0.59
1:D:66:THR:HG22	1:D:67:SER:O	2.02	0.59
1:A:258:LEU:CD1	1:B:251:VAL:HG11	2.31	0.59
1:B:301:GLU:HA	1:B:304:ALA:HB2	1.85	0.59
1:C:357:LEU:O	1:C:358:TYR:HB2	2.02	0.59
1:D:264:ILE:CD1	1:D:279:THR:HG22	2.32	0.59
1:A:447:SER:C	1:A:449:PRO:HD3	2.24	0.59
1:A:101:PHE:O	1:A:105:VAL:HG13	2.03	0.59
1:B:312:VAL:O	1:B:316:LYS:HB2	2.02	0.59
1:D:168:LYS:O	1:D:171:PRO:HD2	2.03	0.59
1:B:135:LEU:HD21	1:B:142:SER:HB2	1.83	0.58
1:D:81:LYS:HG2	1:D:197:VAL:HG13	1.85	0.58
1:A:66:THR:CG2	1:A:70:HIS:HB3	2.34	0.58
1:A:182:LYS:HD2	1:A:218:ALA:HB3	1.84	0.58
1:B:30:PRO:HB2	1:B:332:PRO:HG2	1.85	0.58
1:B:182:LYS:NZ	3:B:1498:NAD:O2B	2.37	0.58
1:C:51:VAL:HG21	1:C:225:HIS:CE1	2.38	0.58
1:C:55:ARG:NH1	4:C:1499:GOL:H31	2.12	0.58
1:C:81:LYS:HD3	1:C:200:GLU:OE1	2.03	0.58
1:D:56:ARG:HD2	1:D:60:ARG:HH12	1.66	0.58
1:D:412:ASN:ND2	1:D:438:GLU:H	2.02	0.58
1:C:3:PHE:CD1	1:C:3:PHE:O	2.56	0.58
1:A:96:ASP:CG	1:A:189:VAL:HG13	2.24	0.58
1:A:365:HIS:H	1:A:365:HIS:CD2	2.21	0.58
1:B:135:LEU:HD21	1:B:142:SER:HB3	1.84	0.58
1:B:306:GLU:O	1:B:310:LYS:HG2	2.04	0.58
1:C:265:VAL:HG22	1:C:422:VAL:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:VAL:HG22	1:A:380:ILE:HD11	1.84	0.58
1:A:304:ALA:O	1:A:308:VAL:HG12	2.03	0.58
1:A:336:LYS:NZ	1:D:116:GLU:OE1	2.35	0.58
1:A:484:GLN:CB	1:B:444:VAL:HB	2.33	0.58
1:A:311:LEU:O	1:A:315:THR:CG2	2.51	0.58
1:B:257[A]:GLU:HB3	3:B:1498:NAD:N7N	2.18	0.58
1:D:373:GLU:O	1:D:374:PRO:C	2.40	0.58
1:A:220:ALA:HB3	1:A:221:PRO:HD3	1.85	0.57
1:A:265:VAL:HG22	1:A:422:VAL:HG23	1.85	0.57
1:B:96:ASP:CG	1:B:189:VAL:HG13	2.24	0.57
1:C:350:LYS:HE3	1:C:356:ILE:HD12	1.85	0.57
1:D:95:ILE:HG22	1:D:324:PHE:CE2	2.38	0.57
1:D:314:TRP:O	1:D:317:ASN:CB	2.52	0.57
1:A:25[B]:ILE:HG23	1:A:26:PRO:HD2	1.86	0.57
1:B:101:PHE:O	1:B:105:VAL:HG13	2.04	0.57
1:C:21:LYS:NZ	5:C:2002:HOH:O	2.37	0.57
1:D:301:GLU:HA	1:D:304:ALA:HB2	1.85	0.57
1:C:105:VAL:CG2	1:C:106:LEU:HD13	2.34	0.57
1:D:30:PRO:HB2	1:D:332:PRO:HG2	1.86	0.57
1:D:101:PHE:O	1:D:105:VAL:HG13	2.04	0.57
1:B:242:LYS:NZ	5:B:2083:HOH:O	2.36	0.57
1:D:377:VAL:HG22	1:D:380:ILE:HD11	1.86	0.57
1:D:414:THR:HG23	5:D:2070:HOH:O	2.03	0.57
1:B:103:GLU:HG2	1:B:285:TRP:HE1	1.69	0.57
1:B:141:LYS:CD	5:B:2051:HOH:O	2.51	0.57
1:C:101:PHE:O	1:C:105:VAL:CG1	2.52	0.57
1:A:301:GLU:HA	1:A:304:ALA:HB2	1.87	0.57
1:A:306:GLU:O	1:A:310:LYS:HG2	2.05	0.57
1:B:95:ILE:HG22	1:B:324:PHE:HE2	1.69	0.57
1:C:308:VAL:O	1:C:311:LEU:HB3	2.03	0.57
1:D:5:ILE:HG22	1:D:6:PRO:N	2.19	0.57
1:D:304:ALA:O	1:D:308:VAL:HG12	2.04	0.57
1:D:308:VAL:O	1:D:312:VAL:HG13	2.04	0.57
1:D:396:LEU:HD11	5:D:2071:HOH:O	2.04	0.57
1:C:490:PRO:HA	1:D:274:LYS:HG2	1.87	0.57
1:D:447:SER:C	1:D:449:PRO:HD3	2.24	0.57
1:B:35:ILE:HG13	1:B:35:ILE:O	2.05	0.57
1:B:268:GLU:CA	1:B:303:ILE:HD11	2.33	0.57
1:B:48:GLU:HG3	5:B:2019:HOH:O	2.04	0.56
1:A:308:VAL:O	1:A:312:VAL:HG13	2.05	0.56
1:B:481:GLN:HE21	1:B:483:THR:HG23	1.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:ASN:ND2	1:C:438:GLU:H	2.03	0.56
1:D:188:SER:HB3	1:D:212:THR:HG21	1.88	0.56
1:C:280:ILE:HG21	1:D:494:TYR:CE2	2.38	0.56
1:D:96:ASP:OD2	1:D:189:VAL:CG1	2.53	0.56
1:A:95:ILE:HB	5:A:2011:HOH:O	2.04	0.56
1:B:81:LYS:HD3	1:B:200:GLU:OE1	2.05	0.56
1:D:406:GLU:O	1:D:410:LEU:HB2	2.05	0.56
1:A:66:THR:HG23	1:A:70:HIS:HB3	1.87	0.56
1:B:3:PHE:CD1	1:B:3:PHE:C	2.77	0.56
1:B:66:THR:HG23	1:B:70:HIS:HB3	1.88	0.56
1:B:141:LYS:HD3	5:B:2051:HOH:O	2.04	0.56
1:D:455:PRO:HG3	1:D:471:TRP:CE3	2.40	0.56
1:D:220:ALA:HB3	1:D:221:PRO:HD3	1.86	0.56
1:D:102:ASP:O	1:D:105:VAL:HG22	2.06	0.56
1:D:268:GLU:CA	1:D:303:ILE:HD11	2.34	0.56
1:A:55:ARG:HD2	1:A:59:ARG:CZ	2.36	0.56
1:B:412:ASN:ND2	1:B:438:GLU:H	2.02	0.56
1:A:444:VAL:HB	1:B:484:GLN:HB3	1.87	0.55
1:A:357:LEU:O	1:A:358:TYR:HB2	2.05	0.55
1:A:381:SER:HB3	1:A:384:MET:HG2	1.89	0.55
1:B:188:SER:HB3	1:B:212:THR:HG21	1.88	0.55
1:C:188:SER:HB3	1:C:212:THR:HG21	1.87	0.55
1:C:301:GLU:HA	1:C:304:ALA:HB2	1.87	0.55
1:B:268:GLU:HA	1:B:303:ILE:CD1	2.34	0.55
1:C:168:LYS:O	1:C:171:PRO:HD2	2.06	0.55
1:D:272:ILE:HD11	1:D:310:LYS:HG3	1.87	0.55
1:D:357:LEU:O	1:D:358:TYR:HB2	2.06	0.55
1:C:30:PRO:HB2	1:C:332:PRO:HG2	1.88	0.55
1:C:225:HIS:HD2	1:C:227:ASP:N	1.94	0.55
1:D:25[B]:ILE:HG23	1:D:26:PRO:HD2	1.87	0.55
1:D:81:LYS:HD3	1:D:200:GLU:OE1	2.07	0.55
1:D:291:CYS:HB3	3:D:1498:NAD:C5N	2.36	0.55
1:C:66:THR:HG23	1:C:70:HIS:HB3	1.88	0.55
1:D:66:THR:HG23	1:D:70:HIS:HB3	1.89	0.55
1:A:264:ILE:CD1	1:A:279:THR:HG22	2.37	0.55
1:C:496:SER:HB3	1:D:314:TRP:CZ2	2.42	0.55
1:A:444:VAL:HB	1:B:484:GLN:HB2	1.88	0.55
1:B:3:PHE:C	1:B:3:PHE:HD1	2.10	0.55
1:B:308:VAL:O	1:B:311:LEU:HB3	2.07	0.55
1:B:344:LYS:O	1:B:348:THR:HG23	2.05	0.55
1:B:455:PRO:HG3	1:B:471:TRP:CE3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:ALA:O	1:C:308:VAL:HG12	2.06	0.55
1:D:363:PRO:O	1:D:364:GLU:CB	2.48	0.55
1:B:48:GLU:HA	1:B:48:GLU:OE1	2.06	0.55
1:A:326:GLU:HG2	1:A:327:GLY:N	2.20	0.54
1:A:95:ILE:HG22	1:A:324:PHE:HE2	1.67	0.54
1:C:60:ARG:O	1:C:62:ASN:N	2.37	0.54
1:C:220:ALA:HB3	1:C:221:PRO:HD3	1.89	0.54
1:B:220:ALA:HB3	1:B:221:PRO:HD3	1.89	0.54
1:B:223:VAL:HA	1:B:231:ILE:HD11	1.89	0.54
1:C:235:GLY:O	1:C:258:LEU:HA	2.07	0.54
1:B:272:ILE:HD11	1:B:310:LYS:HG3	1.87	0.54
1:C:95:ILE:HG22	1:C:324:PHE:HE2	1.70	0.54
1:B:242:LYS:HD3	1:D:486:ILE:HD12	1.90	0.54
1:A:308:VAL:O	1:A:311:LEU:HB3	2.08	0.54
1:B:259:GLY:HA3	3:B:1498:NAD:O2D	2.08	0.54
1:B:260:GLY:HA2	1:B:416:TYR:CG	2.43	0.54
1:B:275:VAL:O	1:B:279:THR:CG2	2.55	0.54
1:B:304:ALA:O	1:B:308:VAL:HG12	2.07	0.54
1:C:308:VAL:O	1:C:312:VAL:HG13	2.08	0.54
1:D:308:VAL:O	1:D:311:LEU:HB3	2.07	0.54
1:D:225:HIS:HD2	1:D:227:ASP:N	1.94	0.54
1:A:268:GLU:OE1	1:A:268:GLU:N	2.29	0.54
1:B:66:THR:HG22	1:B:67:SER:O	2.08	0.54
1:B:76:ARG:HD2	5:B:2012:HOH:O	2.06	0.54
1:C:86:LYS:HE3	5:C:2024:HOH:O	2.08	0.54
1:C:481:GLN:NE2	1:C:483:THR:HG21	2.20	0.54
1:A:214:LEU:CD1	1:D:70:HIS:HB2	2.37	0.53
1:B:481:GLN:NE2	1:B:483:THR:HG21	2.23	0.53
1:A:496:SER:O	1:B:317:ASN:ND2	2.41	0.53
1:B:66:THR:HG21	1:B:70:HIS:CD2	2.42	0.53
1:C:66:THR:CG2	1:C:67:SER:N	2.71	0.53
1:D:396:LEU:CD1	5:D:2071:HOH:O	2.57	0.53
1:A:272:ILE:HG21	1:A:303:ILE:HG21	1.91	0.53
1:A:406:GLU:O	1:A:410:LEU:HB2	2.08	0.53
1:B:155:ILE:HG22	3:B:1498:NAD:H4B	1.90	0.53
1:D:239:THR:HA	1:D:242:LYS:HE3	1.91	0.53
1:D:260:GLY:HA2	1:D:416:TYR:CG	2.44	0.53
1:D:278:TRP:O	1:D:279:THR:C	2.46	0.53
1:B:8:ARG:O	1:B:24:ARG:NH2	2.35	0.53
1:C:264:ILE:CD1	1:C:279:THR:HG22	2.38	0.53
1:A:242:LYS:HE2	1:D:127:GLY:HA3	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:TYR:CD1	1:D:359:GLY:N	2.77	0.53
1:A:272:ILE:HD11	1:A:310:LYS:HG3	1.90	0.53
1:B:257[B]:GLU:HG2	3:B:1498:NAD:H72N	1.74	0.53
1:B:357:LEU:O	1:B:358:TYR:CB	2.56	0.53
1:D:141:LYS:HG3	1:D:486:ILE:HD13	1.91	0.53
1:C:406:GLU:O	1:C:410:LEU:HB2	2.09	0.52
1:B:225:HIS:CD2	1:B:226:PRO:HD2	2.44	0.52
1:D:103:GLU:HG2	1:D:285:TRP:CZ3	2.45	0.52
1:C:223:VAL:HG22	5:C:2051:HOH:O	2.10	0.52
1:C:290:ILE:HB	1:C:293:ALA:HB2	1.91	0.52
1:C:494:TYR:CE2	1:D:280:ILE:HG22	2.44	0.52
1:A:21:LYS:NZ	1:D:61:ASN:HD22	2.07	0.52
1:C:148:PRO:HG3	1:C:175:ALA:O	2.09	0.52
1:D:56:ARG:HD2	1:D:60:ARG:NH1	2.25	0.52
1:A:48:GLU:OE1	1:A:48:GLU:HA	2.08	0.52
1:A:412:ASN:ND2	1:A:438:GLU:H	2.07	0.52
1:B:133:VAL:HG11	5:B:2054:HOH:O	2.09	0.52
1:C:223:VAL:HA	1:C:231:ILE:HD11	1.92	0.52
1:D:66:THR:HG21	1:D:70:HIS:CD2	2.44	0.52
1:B:272:ILE:HG21	1:B:303:ILE:HG21	1.92	0.52
1:B:305:ALA:O	1:B:306:GLU:CB	2.56	0.52
1:A:102:ASP:O	1:A:105:VAL:HG22	2.09	0.52
1:D:76:ARG:CG	1:D:76:ARG:NH1	2.71	0.52
1:D:348:THR:O	1:D:352:GLU:HG3	2.10	0.52
1:D:4:PRO:O	1:D:5:ILE:C	2.49	0.52
1:D:305:ALA:O	1:D:306:GLU:HB3	2.09	0.52
1:D:381:SER:HB3	1:D:384:MET:HG2	1.91	0.52
1:B:271:ASP:OD1	1:B:274:LYS:HD2	2.09	0.51
1:D:5:ILE:N	1:D:5:ILE:HD12	2.26	0.51
1:A:188:SER:HB3	1:A:212:THR:HG21	1.93	0.51
1:A:412:ASN:HD21	1:A:438:GLU:H	1.58	0.51
1:A:439:VAL:HG13	1:A:441:ALA:H	1.76	0.51
1:B:186:LEU:O	1:B:187:ALA:HB2	2.11	0.51
1:B:414:THR:CG2	5:B:2108:HOH:O	2.55	0.51
1:C:95:ILE:HA	5:C:2009:HOH:O	2.08	0.51
1:D:272:ILE:O	1:D:272:ILE:HG13	2.09	0.51
1:D:279:THR:HG21	1:D:307:PHE:HZ	1.75	0.51
1:C:5:ILE:HG22	1:C:6:PRO:N	2.24	0.51
1:D:160:TYR:CE1	4:D:1500:GOL:H32	2.46	0.51
1:D:447:SER:O	1:D:448:GLN:HB2	2.11	0.51
1:A:178:THR:HG22	1:A:207:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLY:O	1:A:258:LEU:HA	2.10	0.51
1:C:260:GLY:HA2	1:C:416:TYR:CG	2.45	0.51
1:D:300:HIS:ND1	1:D:302:SER:HB2	2.26	0.51
1:A:300:HIS:ND1	1:A:302:SER:HB2	2.25	0.51
1:A:35:ILE:HG13	1:A:35:ILE:O	2.08	0.51
1:C:279:THR:HG21	1:C:307:PHE:HZ	1.76	0.51
1:D:96:ASP:O	1:D:96:ASP:OD1	2.29	0.51
1:C:29:ASN:HB2	1:C:36:ILE:HD13	1.93	0.51
1:D:272:ILE:HG21	1:D:303:ILE:HG21	1.92	0.51
1:A:481:GLN:NE2	1:A:483:THR:HG21	2.18	0.51
1:A:481:GLN:HE21	1:A:483:THR:HG23	1.74	0.51
1:C:257[B]:GLU:HB3	3:C:1498:NAD:C7N	2.41	0.50
1:C:444:VAL:HB	1:D:484:GLN:HB3	1.93	0.50
1:D:58:PHE:CE1	1:D:150:GLY:HA2	2.46	0.50
1:D:235:GLY:O	1:D:258:LEU:HA	2.11	0.50
1:C:66:THR:HG21	1:C:70:HIS:CD2	2.45	0.50
1:D:4:PRO:O	1:D:5:ILE:O	2.30	0.50
1:D:225:HIS:CD2	1:D:226:PRO:HD2	2.46	0.50
1:A:5:ILE:H	1:A:6:PRO:CD	2.20	0.50
1:A:5:ILE:O	1:A:6:PRO:O	2.29	0.50
1:A:348:THR:HG22	1:C:134:THR:OG1	2.12	0.50
1:A:481:GLN:NE2	5:A:2157:HOH:O	2.41	0.50
1:C:15:GLU:HG2	1:C:17:ARG:NH1	2.19	0.50
1:C:381:SER:HB3	1:C:384:MET:HG2	1.93	0.50
1:D:186:LEU:O	1:D:187:ALA:HB2	2.11	0.50
1:D:291:CYS:SG	3:D:1498:NAD:C4N	2.99	0.50
1:C:6:PRO:HG2	1:C:92:LEU:HD13	1.93	0.50
1:C:225:HIS:CD2	1:C:226:PRO:HD2	2.46	0.50
1:C:272:ILE:CD1	1:C:306:GLU:HG2	2.42	0.50
1:D:85:LYS:NZ	1:D:200:GLU:OE2	2.45	0.50
1:D:223:VAL:HA	1:D:231:ILE:HD11	1.94	0.50
1:D:264:ILE:HD11	1:D:279:THR:HG22	1.94	0.50
1:D:481:GLN:NE2	1:D:483:THR:HG21	2.21	0.50
1:A:5:ILE:N	1:A:6:PRO:CD	2.74	0.50
1:B:66:THR:HG21	1:B:70:HIS:HD2	1.76	0.50
1:C:186:LEU:O	1:C:187:ALA:HB2	2.11	0.50
1:C:474:GLN:NE2	5:C:2122:HOH:O	2.42	0.50
1:A:148:PRO:HG3	1:A:175:ALA:O	2.12	0.50
1:B:5:ILE:HG22	1:B:5:ILE:O	2.06	0.50
1:C:48:GLU:OE1	1:C:48:GLU:HA	2.12	0.50
1:B:182:LYS:C	1:B:182:LYS:HE2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:HG13	1:C:37:GLY:C	2.32	0.50
1:C:478:ASN:ND2	1:D:466:ARG:HH21	2.09	0.50
1:D:282:GLY:HA2	1:D:448:GLN:CG	2.42	0.49
1:D:290:ILE:HB	1:D:293:ALA:HB2	1.94	0.49
1:C:51:VAL:HG23	1:C:52:VAL:N	2.27	0.49
1:A:362:ARG:HG3	1:A:362:ARG:HH11	1.77	0.49
1:C:160:TYR:HB2	1:C:164:MET:HG2	1.94	0.49
1:A:282:GLY:HA2	1:A:448:GLN:CG	2.43	0.49
1:A:348:THR:O	1:A:352:GLU:HG3	2.12	0.49
1:C:10:LEU:HD13	1:C:211:LEU:HD22	1.94	0.49
1:C:15:GLU:CD	1:C:17:ARG:NH1	2.66	0.49
1:C:315:THR:HG21	1:C:376:ILE:HD11	1.95	0.49
1:C:438:GLU:HG2	4:D:1502:GOL:H31	1.94	0.49
1:A:386:ILE:HB	5:A:2113:HOH:O	2.13	0.49
1:B:235:GLY:O	1:B:258:LEU:HA	2.12	0.49
1:D:3:PHE:CZ	1:D:324:PHE:CZ	2.98	0.49
1:A:484:GLN:HB3	1:B:444:VAL:HB	1.94	0.49
1:D:148:PRO:HG3	1:D:176:GLY:HA3	1.95	0.49
1:A:182:LYS:HG2	1:A:211:LEU:O	2.13	0.49
1:C:268:GLU:HA	1:C:303:ILE:CD1	2.38	0.49
1:C:348:THR:O	1:C:352:GLU:HG3	2.12	0.49
1:C:392:PHE:CE1	3:C:1498:NAD:H2D	2.48	0.49
1:B:141:LYS:HG2	5:B:2051:HOH:O	2.13	0.49
1:B:257[B]:GLU:HG2	3:B:1498:NAD:N7N	2.28	0.49
1:B:447:SER:O	1:B:448:GLN:HB2	2.13	0.49
1:C:62:ASN:OD1	1:C:62:ASN:O	2.31	0.49
1:A:223:VAL:HA	1:A:231:ILE:HD11	1.93	0.49
1:C:291:CYS:HB3	3:C:1498:NAD:C6N	2.42	0.49
1:A:290:ILE:HB	1:A:293:ALA:HB2	1.93	0.48
1:B:7:ALA:O	1:B:8:ARG:HD3	2.12	0.48
1:B:148:PRO:HG3	1:B:176:GLY:HA3	1.95	0.48
1:D:95:ILE:CG2	1:D:324:PHE:HZ	2.21	0.48
1:D:160:TYR:HB2	1:D:164:MET:HG2	1.94	0.48
1:D:261:LYS:HG3	1:D:296:ARG:HD3	1.95	0.48
1:A:98:GLY:O	1:A:332:PRO:HD2	2.13	0.48
1:A:314:TRP:CZ2	1:B:496:SER:HB3	2.48	0.48
1:B:272:ILE:O	1:B:272:ILE:HG13	2.13	0.48
1:C:257[B]:GLU:HG2	3:C:1498:NAD:O7N	2.12	0.48
1:C:439:VAL:HG13	1:C:441:ALA:H	1.77	0.48
1:A:264:ILE:HD13	1:A:279:THR:HG22	1.93	0.48
1:B:29:ASN:HB2	1:B:36:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:THR:HG21	1:C:70:HIS:HD2	1.78	0.48
1:C:182:LYS:HE2	1:C:182:LYS:C	2.32	0.48
1:A:260:GLY:HA2	1:A:416:TYR:CG	2.48	0.48
1:A:272:ILE:HG13	1:A:272:ILE:O	2.12	0.48
1:A:29:ASN:HB2	1:A:36:ILE:HD13	1.95	0.48
1:B:160:TYR:HB2	1:B:164:MET:HG2	1.95	0.48
1:C:96:ASP:CG	1:C:189:VAL:HG13	2.31	0.48
1:D:239:THR:O	1:D:243:VAL:HG13	2.13	0.48
1:D:320:ILE:O	1:D:365:HIS:HE1	1.97	0.48
1:A:66:THR:CG2	1:A:67:SER:N	2.76	0.48
1:B:225:HIS:HD2	1:B:227:ASP:N	1.96	0.48
1:C:76:ARG:NH1	1:C:76:ARG:CG	2.69	0.48
1:C:148:PRO:HG3	1:C:176:GLY:HA3	1.95	0.48
1:B:271:ASP:OD2	1:B:274:LYS:CD	2.62	0.48
1:C:11:PHE:CZ	1:C:14:GLY:HA2	2.49	0.48
1:D:146:ARG:HG2	1:D:479:ILE:HD13	1.95	0.48
1:A:3:PHE:O	1:A:4:PRO:O	2.32	0.48
1:A:27:VAL:HG13	1:A:37:GLY:C	2.34	0.48
1:A:276:VAL:HG11	1:A:314:TRP:CD1	2.49	0.48
1:B:257[B]:GLU:OE2	1:B:456:TRP:O	2.31	0.48
1:B:242:LYS:HD3	1:D:486:ILE:CD1	2.44	0.48
1:C:60:ARG:HB3	1:C:62:ASN:HB3	1.95	0.48
1:B:86:LYS:O	1:B:90:VAL:HG12	2.14	0.48
1:C:448:GLN:N	1:C:449:PRO:CD	2.76	0.48
1:D:315:THR:HG21	1:D:376:ILE:HD11	1.96	0.48
1:A:51:VAL:HG21	1:A:225:HIS:NE2	2.28	0.47
1:B:182:LYS:HG2	1:B:211:LEU:O	2.14	0.47
1:A:62:ASN:OD1	1:A:62:ASN:O	2.32	0.47
1:D:48:GLU:HA	1:D:48:GLU:OE1	2.13	0.47
1:D:159:ASN:HD21	3:D:1498:NAD:H5N	1.79	0.47
1:A:182:LYS:C	1:A:182:LYS:HE2	2.35	0.47
1:A:256:LEU:HB3	1:A:258:LEU:HD21	1.97	0.47
1:B:76:ARG:CG	1:B:76:ARG:NH1	2.71	0.47
1:C:106:LEU:HD12	1:C:106:LEU:HA	1.54	0.47
1:C:280:ILE:CG2	1:D:494:TYR:CD2	2.93	0.47
1:A:225:HIS:HD2	1:A:227:ASP:N	1.96	0.47
1:D:135:LEU:HD21	1:D:142:SER:HB2	1.93	0.47
1:A:279:THR:HG21	1:A:307:PHE:HZ	1.79	0.47
1:B:282:GLY:HA2	1:B:448:GLN:CG	2.44	0.47
1:C:239:THR:O	1:C:243:VAL:HG13	2.15	0.47
1:D:3:PHE:HZ	1:D:95:ILE:CG2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:O	1:A:90:VAL:HG12	2.14	0.47
1:A:466:ARG:HH21	1:B:478:ASN:ND2	2.12	0.47
1:C:15:GLU:CG	1:C:17:ARG:NH1	2.76	0.47
1:C:35:ILE:O	1:C:35:ILE:HG13	2.15	0.47
1:C:60:ARG:C	1:C:62:ASN:H	2.17	0.47
1:C:98:GLY:O	1:C:332:PRO:HD2	2.15	0.47
1:D:481:GLN:HE21	1:D:483:THR:HG23	1.75	0.47
1:A:58:PHE:CE1	1:A:150:GLY:HA2	2.50	0.47
1:A:358:TYR:CD1	1:A:359:GLY:N	2.83	0.47
1:B:279:THR:HG21	1:B:307:PHE:HZ	1.80	0.47
1:C:86:LYS:O	1:C:90:VAL:HG12	2.15	0.47
1:D:3:PHE:CB	1:D:4:PRO:CD	2.92	0.47
1:A:66:THR:HG21	1:A:70:HIS:CD2	2.50	0.47
1:A:225:HIS:HA	1:A:226:PRO:HD3	1.71	0.47
1:B:102:ASP:O	1:B:105:VAL:HG22	2.14	0.47
1:B:229:ASP:O	1:B:253:PRO:HD2	2.14	0.47
1:C:303:ILE:H	1:C:303:ILE:HG13	1.48	0.47
1:C:444:VAL:HB	1:D:484:GLN:HB2	1.96	0.47
1:D:362:ARG:HG3	1:D:362:ARG:HH11	1.79	0.47
1:A:25[B]:ILE:HD11	1:A:214:LEU:HD11	1.97	0.47
1:C:66:THR:HG22	1:C:67:SER:N	2.30	0.47
1:B:27:VAL:HG13	1:B:37:GLY:C	2.36	0.46
1:B:58:PHE:CE1	1:B:150:GLY:HA2	2.50	0.46
1:B:261:LYS:CG	1:B:296:ARG:HD2	2.44	0.46
1:C:48:GLU:OE1	1:C:48:GLU:CA	2.64	0.46
1:C:276:VAL:HG11	1:C:314:TRP:CD1	2.50	0.46
1:A:196:GLU:O	1:A:197:VAL:C	2.54	0.46
1:A:225:HIS:O	1:A:252:LYS:NZ	2.49	0.46
1:A:306:GLU:CG	1:A:310:LYS:NZ	2.78	0.46
1:B:3:PHE:HD1	1:B:4:PRO:HD3	1.78	0.46
1:B:12:ILE:HD11	1:B:211:LEU:HD21	1.96	0.46
1:B:448:GLN:N	1:B:449:PRO:CD	2.78	0.46
1:B:48:GLU:OE1	1:B:48:GLU:CA	2.63	0.46
1:B:95:ILE:HG22	1:B:324:PHE:HZ	1.78	0.46
1:B:281:PHE:O	1:B:285:TRP:HB3	2.15	0.46
1:A:182:LYS:NZ	3:A:1498:NAD:O2B	2.48	0.46
1:A:229:ASP:O	1:A:253:PRO:HD2	2.16	0.46
1:B:66:THR:CG2	1:B:67:SER:N	2.78	0.46
1:B:290:ILE:HB	1:B:293:ALA:HB2	1.96	0.46
1:D:283:CYS:SG	1:D:396:LEU:HD23	2.56	0.46
1:A:76:ARG:CG	1:A:76:ARG:NH1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:PHE:HD2	5:C:2077:HOH:O	1.97	0.46
1:C:358:TYR:CD1	1:C:359:GLY:N	2.83	0.46
1:D:51:VAL:HG21	1:D:225:HIS:NE2	2.31	0.46
1:D:256:LEU:HB3	1:D:258:LEU:HD21	1.97	0.46
1:B:315:THR:HG21	1:B:376:ILE:HD11	1.97	0.46
1:C:5:ILE:CG2	1:C:6:PRO:CD	2.81	0.46
1:C:466:ARG:HH21	1:D:478:ASN:ND2	2.13	0.46
1:D:12:ILE:HD11	1:D:211:LEU:HD21	1.98	0.46
1:B:91:LYS:O	1:B:95:ILE:HG23	2.16	0.46
1:B:348:THR:O	1:B:352:GLU:HG3	2.14	0.46
1:B:350:LYS:HE3	1:B:356:ILE:CD1	2.43	0.46
1:A:148:PRO:HG3	1:A:176:GLY:HA3	1.98	0.46
1:C:278:TRP:CH2	1:D:491:TRP:CD2	3.04	0.46
1:C:362:ARG:HG3	1:C:362:ARG:HH11	1.80	0.46
1:C:487:SER:O	1:C:488:ASP:CB	2.62	0.46
1:C:229:ASP:O	1:C:253:PRO:HD2	2.16	0.46
1:D:268:GLU:HA	1:D:303:ILE:CD1	2.36	0.46
1:A:181:LEU:HD13	1:A:183:PRO:HG3	1.97	0.45
1:A:447:SER:O	1:A:448:GLN:HB2	2.15	0.45
1:B:98:GLY:O	1:B:332:PRO:HD2	2.16	0.45
1:B:242:LYS:HG2	1:D:486:ILE:HD12	1.97	0.45
1:B:276:VAL:HG11	1:B:314:TRP:CD1	2.51	0.45
1:C:264:ILE:HD13	1:C:279:THR:HG22	1.98	0.45
1:C:357:LEU:O	1:C:358:TYR:CB	2.65	0.45
1:D:276:VAL:HG11	1:D:314:TRP:CD1	2.51	0.45
1:D:401:PHE:CD2	1:D:407:ALA:HB2	2.51	0.45
1:D:264:ILE:HG23	1:D:297:LEU:HA	1.99	0.45
1:D:414:THR:HB	1:D:416:TYR:H	1.82	0.45
1:A:8:ARG:O	1:A:24:ARG:NH2	2.30	0.45
1:A:262:SER:HA	1:A:263:PRO:HD3	1.87	0.45
1:A:320:ILE:O	1:A:365:HIS:HE1	1.99	0.45
1:B:215:GLY:HA3	3:B:1498:NAD:C8A	2.47	0.45
1:C:6:PRO:CB	1:C:193:GLU:OE2	2.62	0.45
1:C:51:VAL:CG2	1:C:52:VAL:N	2.79	0.45
1:C:268:GLU:CA	1:C:303:ILE:HD11	2.38	0.45
1:C:282:GLY:HA2	1:C:448:GLN:CG	2.47	0.45
1:D:358:TYR:CD1	1:D:358:TYR:C	2.90	0.45
1:D:264:ILE:HD13	1:D:279:THR:HG22	1.97	0.45
1:D:448:GLN:N	1:D:449:PRO:CD	2.79	0.45
1:A:280:ILE:HD11	1:A:311:LEU:HD12	1.98	0.45
1:B:108:ILE:HA	1:B:111:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:LYS:HG2	1:D:211:LEU:O	2.17	0.45
1:A:8:ARG:HG3	1:A:9:GLN:H	1.81	0.45
1:A:35:ILE:O	1:A:35:ILE:CG1	2.65	0.45
1:A:341:LYS:CE	5:A:2110:HOH:O	2.49	0.45
1:A:448:GLN:N	1:A:449:PRO:CD	2.79	0.45
1:B:103:GLU:OE2	1:B:285:TRP:HD1	2.00	0.45
1:B:146:ARG:HG2	1:B:479:ILE:HD13	1.99	0.45
1:B:264:ILE:HG21	5:B:2091:HOH:O	2.16	0.45
1:B:29:ASN:OD1	1:B:30:PRO:HD2	2.17	0.45
1:B:403:SER:OG	1:B:405:ASP:OD1	2.33	0.45
1:C:3:PHE:CD1	1:C:3:PHE:N	2.84	0.45
1:D:93:GLU:OE1	1:D:190:THR:OG1	2.24	0.45
1:A:309:ASP:O	1:A:312:VAL:HG22	2.17	0.45
1:C:481:GLN:HE21	1:C:483:THR:HG23	1.74	0.45
1:D:346:ILE:HG23	1:D:356:ILE:HD11	1.99	0.45
1:A:5:ILE:N	1:A:6:PRO:HD3	2.17	0.44
1:A:48:GLU:OE1	1:A:48:GLU:CA	2.64	0.44
1:B:282:GLY:HA2	1:B:448:GLN:HG2	1.99	0.44
1:D:66:THR:CG2	1:D:67:SER:N	2.80	0.44
1:D:89:PHE:HB3	1:D:108:ILE:HD12	1.98	0.44
1:D:229:ASP:O	1:D:253:PRO:HD2	2.17	0.44
1:D:350:LYS:HE3	1:D:356:ILE:HD12	1.98	0.44
1:D:392:PHE:O	5:D:2069:HOH:O	2.21	0.44
1:D:478:ASN:ND2	1:D:478:ASN:C	2.70	0.44
1:A:160:TYR:HB2	1:A:164:MET:HG2	1.99	0.44
1:A:239:THR:O	1:A:243:VAL:HG13	2.17	0.44
1:A:257[B]:GLU:HB3	3:A:1498:NAD:C7N	2.47	0.44
1:A:362:ARG:HG3	1:A:362:ARG:NH1	2.32	0.44
1:D:3:PHE:HB3	1:D:91:LYS:NZ	2.32	0.44
1:D:282:GLY:HA2	1:D:448:GLN:HG2	1.98	0.44
1:A:261:LYS:HG3	1:A:296:ARG:HD3	1.98	0.44
1:C:451:PHE:CZ	1:D:137:MET:HG3	2.51	0.44
1:A:478:ASN:ND2	1:B:466:ARG:HH21	2.15	0.44
1:A:484:GLN:HB2	1:B:444:VAL:HB	1.99	0.44
1:B:362:ARG:HG3	1:B:362:ARG:HH11	1.82	0.44
1:D:261:LYS:CG	1:D:296:ARG:HD2	2.46	0.44
1:C:5:ILE:HA	1:C:6:PRO:HD3	1.81	0.44
1:D:96:ASP:OD2	1:D:189:VAL:HG13	2.17	0.44
1:D:401:PHE:HD2	1:D:403:SER:O	2.01	0.44
1:D:439:VAL:HG13	1:D:441:ALA:H	1.82	0.44
1:D:450[A]:CYS:O	4:D:1501:GOL:H12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:CYS:HB3	3:B:1498:NAD:C6N	2.48	0.44
1:C:112:ALA:O	1:C:116:GLU:HG3	2.18	0.44
1:C:429:ARG:HA	1:C:432:ARG:HH21	1.77	0.44
1:C:51:VAL:HG21	1:C:225:HIS:NE2	2.32	0.44
1:C:139:ARG:HH12	1:C:489:GLU:HB2	1.83	0.44
1:D:5:ILE:CG2	1:D:6:PRO:N	2.79	0.44
1:A:103:GLU:HG2	1:A:285:TRP:HE1	1.82	0.44
1:A:251:VAL:HG13	1:B:256:LEU:HD12	1.99	0.44
1:C:280:ILE:HG21	1:D:494:TYR:CD2	2.53	0.44
1:D:9:GLN:NE2	1:D:24:ARG:NH2	2.64	0.44
1:D:193:GLU:OE1	1:D:193:GLU:HA	2.18	0.44
1:A:152:VAL:HG23	1:A:154:LEU:HD21	1.99	0.44
1:B:112:ALA:O	1:B:116:GLU:HG3	2.18	0.44
1:B:256:LEU:HB3	1:B:258:LEU:HD21	1.99	0.44
1:B:261:LYS:HG3	1:B:296:ARG:HD3	1.97	0.44
1:D:170:ALA:HB3	1:D:171:PRO:HD3	2.00	0.44
1:D:429:ARG:O	1:D:433:ILE:HG12	2.18	0.44
1:A:21:LYS:HG3	1:A:43:THR:HG21	2.00	0.43
1:A:186:LEU:O	1:A:187:ALA:HB2	2.18	0.43
1:D:66:THR:HG21	1:D:70:HIS:HD2	1.80	0.43
1:D:108:ILE:HA	1:D:111:VAL:HG13	2.00	0.43
1:A:495:LYS:HG2	5:A:2163:HOH:O	2.18	0.43
1:B:264:ILE:HG23	1:B:297:LEU:HA	2.00	0.43
1:C:320:ILE:O	1:C:365:HIS:HE1	2.01	0.43
1:A:168:LYS:C	1:A:171:PRO:HD2	2.39	0.43
1:A:268:GLU:HA	1:A:303:ILE:CD1	2.44	0.43
1:B:401:PHE:CD2	1:B:407:ALA:HB2	2.53	0.43
1:C:99:LYS:HB3	1:C:99:LYS:HE2	1.76	0.43
1:D:152:VAL:HG23	1:D:154:LEU:HD21	2.01	0.43
1:D:309:ASP:O	1:D:312:VAL:HG22	2.18	0.43
1:B:139:ARG:HH12	1:B:489:GLU:HB2	1.83	0.43
1:B:262:SER:HA	1:B:263:PRO:HD3	1.91	0.43
1:A:312:VAL:O	1:A:316:LYS:HB2	2.18	0.43
1:B:168:LYS:C	1:B:171:PRO:HD2	2.39	0.43
1:B:297:LEU:HB2	1:B:396:LEU:HD11	2.00	0.43
1:D:257[B]:GLU:HB3	3:D:1498:NAD:C7N	2.49	0.43
1:D:447:SER:O	1:D:448:GLN:CB	2.66	0.43
1:A:12:ILE:HD11	1:A:211:LEU:HD21	1.99	0.43
1:A:91:LYS:O	1:A:95:ILE:HG23	2.17	0.43
1:A:225:HIS:CD2	1:A:226:PRO:HD2	2.53	0.43
1:A:252:LYS:HE3	1:A:252:LYS:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ILE:HG23	1:A:356:ILE:HD11	2.00	0.43
1:A:378:THR:HG22	1:A:398:VAL:HB	2.01	0.43
1:C:401:PHE:HD2	1:C:403:SER:O	2.02	0.43
1:D:110:ASP:CG	4:D:1501:GOL:H2	2.35	0.43
1:A:137:MET:HB3	5:A:2044:HOH:O	2.19	0.43
1:B:94:THR:HG23	1:B:99:LYS:O	2.18	0.43
1:B:280:ILE:HD11	1:B:311:LEU:HD12	2.00	0.43
1:C:122:ALA:HB2	1:C:174:ALA:HB1	2.01	0.43
1:D:136:PRO:O	1:D:137:MET:C	2.55	0.43
1:D:401:PHE:CE2	1:D:407:ALA:HB2	2.54	0.43
1:C:58:PHE:CE1	1:C:150:GLY:HA2	2.54	0.43
1:C:358:TYR:CD1	1:C:358:TYR:C	2.92	0.43
1:D:98:GLY:O	1:D:332:PRO:HD2	2.19	0.43
1:A:131:ALA:HA	1:A:132:PRO:HD3	1.86	0.43
1:A:262:SER:HB3	1:A:419:ALA:O	2.19	0.43
1:A:300:HIS:O	1:A:301:GLU:C	2.58	0.43
1:A:391:VAL:HB	5:A:2126:HOH:O	2.19	0.43
1:B:5:ILE:HG23	1:B:6:PRO:HD2	2.00	0.43
1:C:359:GLY:HA2	1:C:373:GLU:OE1	2.19	0.43
1:D:272:ILE:HD12	1:D:307:PHE:CA	2.41	0.43
1:C:30:PRO:HG2	1:C:98:GLY:HA3	2.00	0.43
1:C:272:ILE:HG21	1:C:303:ILE:HG21	2.00	0.43
1:C:390[A]:GLU:HG3	5:C:2065:HOH:O	2.18	0.43
1:D:48:GLU:OE1	1:D:48:GLU:CA	2.67	0.43
1:D:303:ILE:H	1:D:303:ILE:HG13	1.53	0.43
1:A:280:ILE:HG21	1:A:318:ILE:HD11	2.00	0.42
1:A:282:GLY:HA2	1:A:448:GLN:HG2	2.00	0.42
1:A:348:THR:HG22	1:C:134:THR:CG2	2.49	0.42
1:B:252:LYS:HE3	1:B:252:LYS:HB2	1.75	0.42
1:B:439:VAL:HG13	1:B:441:ALA:H	1.84	0.42
1:C:9:GLN:HB3	1:C:17:ARG:O	2.19	0.42
1:D:137:MET:H	1:D:137:MET:HG2	1.54	0.42
1:D:482:VAL:O	1:D:482:VAL:HG22	2.19	0.42
1:B:62[A]:ASN:OD1	1:B:62[A]:ASN:O	2.37	0.42
1:C:60:ARG:C	1:C:62:ASN:N	2.72	0.42
1:C:193:GLU:HA	1:C:193:GLU:OE1	2.20	0.42
1:C:225:HIS:HA	1:C:226:PRO:HD3	1.76	0.42
1:C:314:TRP:CZ2	1:D:496:SER:HB3	2.54	0.42
1:D:3:PHE:HB2	1:D:4:PRO:CD	2.49	0.42
1:D:278:TRP:O	1:D:280:ILE:N	2.52	0.42
1:A:357:LEU:O	1:A:358:TYR:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:TYR:CD1	1:B:358:TYR:C	2.93	0.42
1:C:105:VAL:CG2	1:C:106:LEU:N	2.83	0.42
1:D:262:SER:HA	1:D:263:PRO:HD3	1.89	0.42
1:D:357:LEU:O	1:D:357:LEU:CD2	2.67	0.42
1:A:129:GLN:O	1:A:130:LYS:HB2	2.20	0.42
1:C:264:ILE:HD11	1:C:279:THR:HG22	2.01	0.42
1:C:362:ARG:HG3	1:C:362:ARG:NH1	2.34	0.42
3:C:1498:NAD:H8A	3:C:1498:NAD:H2B	1.80	0.42
1:D:139:ARG:HH12	1:D:489:GLU:HB2	1.85	0.42
1:D:493:TRP:HD1	1:D:494:TYR:CD1	2.37	0.42
1:B:35:ILE:O	1:B:35:ILE:CG1	2.65	0.42
1:C:108:ILE:HA	1:C:111:VAL:HG13	2.01	0.42
1:C:272:ILE:HG21	1:C:272:ILE:HD13	1.79	0.42
1:D:305:ALA:O	1:D:306:GLU:HB2	2.18	0.42
1:D:330:LEU:HD22	1:D:331:GLY:O	2.20	0.42
1:B:3:PHE:CD1	1:B:3:PHE:O	2.73	0.42
1:C:130:LYS:HA	1:C:143:HIS:CD2	2.54	0.42
1:C:264:ILE:HG23	1:C:297:LEU:HA	2.01	0.42
1:C:447:SER:O	1:C:448:GLN:HB2	2.19	0.42
1:D:125:LEU:O	1:D:128:LYS:HB2	2.20	0.42
1:A:264:ILE:HG23	1:A:297:LEU:HA	2.02	0.42
1:A:315:THR:HG21	1:A:376:ILE:HD11	2.02	0.42
1:B:362:ARG:HG3	1:B:362:ARG:NH1	2.35	0.42
1:C:3:PHE:O	1:C:3:PHE:HD1	2.00	0.42
1:D:362:ARG:HG3	1:D:362:ARG:NH1	2.35	0.42
1:A:358:TYR:CD1	1:A:358:TYR:C	2.93	0.42
1:C:181:LEU:HD13	1:C:183:PRO:HG3	2.01	0.42
1:C:182:LYS:HG2	1:C:211:LEU:O	2.19	0.42
1:A:30:PRO:HG2	1:A:98:GLY:HA3	2.02	0.42
1:A:121:GLN:NE2	5:A:2038:HOH:O	2.53	0.42
1:B:205:PRO:HD2	5:B:2022:HOH:O	2.19	0.42
1:B:264:ILE:HA	1:B:421:ALA:O	2.19	0.42
1:C:251[A]:VAL:HG13	1:D:256:LEU:HD12	2.02	0.42
1:C:350:LYS:HE3	1:C:356:ILE:CD1	2.49	0.42
1:D:12:ILE:HG21	1:D:49:VAL:HG23	2.02	0.42
1:D:62:ASN:OD1	1:D:62:ASN:O	2.37	0.42
1:D:182:LYS:C	1:D:182:LYS:HE2	2.40	0.42
1:D:306:GLU:O	1:D:307:PHE:C	2.57	0.42
1:A:256:LEU:HD12	1:B:251:VAL:HG13	2.02	0.41
1:A:261:LYS:CG	1:A:296:ARG:HD2	2.45	0.41
1:A:264:ILE:HA	1:A:421:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:PHE:CD2	1:A:445:ASN:HA	2.55	0.41
1:B:257[A]:GLU:OE2	1:B:467:GLU:HG3	2.20	0.41
1:B:257[B]:GLU:CG	3:B:1498:NAD:H72N	2.33	0.41
1:B:283:CYS:SG	1:B:396:LEU:HD23	2.60	0.41
1:B:381:SER:HG	1:B:383[A]:SER:HB2	1.84	0.41
1:B:359:GLY:HA2	1:B:373:GLU:OE1	2.20	0.41
1:C:3:PHE:N	1:C:3:PHE:HD1	2.18	0.41
1:A:251:VAL:O	1:A:251:VAL:CG1	2.67	0.41
1:C:252:LYS:HE3	1:C:252:LYS:HB2	1.82	0.41
1:D:268:GLU:HG2	1:D:269:ASP:N	2.34	0.41
1:A:139:ARG:HH12	1:A:489:GLU:HB2	1.85	0.41
1:B:143:HIS:CE1	1:B:482:VAL:HG22	2.55	0.41
1:B:357:LEU:O	1:B:357:LEU:CD2	2.66	0.41
1:C:125:LEU:O	1:C:128:LYS:HB2	2.19	0.41
1:D:262:SER:HB3	1:D:419:ALA:O	2.21	0.41
1:C:280:ILE:HD11	1:C:311:LEU:HD12	2.02	0.41
1:C:434:THR:HB	1:C:442:VAL:HG11	2.02	0.41
1:D:58:PHE:CZ	1:D:150:GLY:HA2	2.56	0.41
1:B:12:ILE:HG21	1:B:49:VAL:HG23	2.03	0.41
1:D:182:LYS:HD2	1:D:218:ALA:CB	2.47	0.41
1:B:152:VAL:HG23	1:B:154:LEU:HD21	2.03	0.41
1:C:47:VAL:O	1:C:51:VAL:HG13	2.21	0.41
1:D:30:PRO:HG2	1:D:98:GLY:HA3	2.03	0.41
1:A:264:ILE:HG23	1:A:264:ILE:O	2.20	0.41
1:A:494:TYR:CZ	1:B:280:ILE:HG22	2.55	0.41
1:B:143:HIS:CE1	1:B:482:VAL:CG2	3.04	0.41
1:B:346:ILE:HG23	1:B:356:ILE:HD11	2.03	0.41
1:B:423:PHE:CD2	1:B:445:ASN:HA	2.56	0.41
1:D:357:LEU:O	1:D:358:TYR:CB	2.68	0.41
1:A:429:ARG:O	1:A:433:ILE:HG12	2.21	0.41
1:B:203:LEU:HD23	1:B:203:LEU:HA	1.82	0.41
1:B:271:ASP:OD2	1:B:274:LYS:CE	2.68	0.41
1:C:182:LYS:CE	1:C:183:PRO:O	2.69	0.41
1:C:262:SER:HA	1:C:263:PRO:HD3	1.86	0.41
1:C:315:THR:HA	1:C:318:ILE:HD12	2.03	0.41
1:C:346:ILE:HG23	1:C:356:ILE:HD11	2.02	0.41
1:C:378:THR:HG22	1:C:398:VAL:HB	2.02	0.41
1:D:171:PRO:HB2	1:D:476:TYR:CE2	2.55	0.41
1:D:264:ILE:HA	1:D:421:ALA:O	2.20	0.41
1:A:447:SER:O	1:A:448:GLN:CB	2.69	0.41
1:B:239:THR:O	1:B:243:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LYS:HA	1:B:143:HIS:CD2	2.56	0.40
1:B:268:GLU:HG2	1:B:269:ASP:N	2.37	0.40
1:C:423:PHE:CD2	1:C:445:ASN:HA	2.56	0.40
1:C:478:ASN:ND2	1:C:478:ASN:C	2.75	0.40
1:D:83:THR:O	1:D:86:LYS:HB2	2.21	0.40
1:D:168:LYS:C	1:D:171:PRO:HD2	2.41	0.40
1:D:306:GLU:O	1:D:309:ASP:N	2.54	0.40
1:D:482:VAL:O	1:D:482:VAL:CG2	2.69	0.40
1:A:112:ALA:O	1:A:116:GLU:HG3	2.21	0.40
1:A:281:PHE:O	1:A:285:TRP:HB3	2.21	0.40
1:A:330:LEU:HD22	1:A:331:GLY:O	2.22	0.40
1:C:131:ALA:HA	1:C:132:PRO:HD3	1.90	0.40
1:C:250:LEU:C	1:C:251[B]:VAL:HG22	2.42	0.40
1:C:309:ASP:O	1:C:312:VAL:HG22	2.20	0.40
1:C:439:VAL:HG13	1:C:440:GLY:N	2.36	0.40
1:C:484:GLN:CB	1:D:444:VAL:HB	2.51	0.40
1:D:434:THR:HB	1:D:442:VAL:HG11	2.03	0.40
1:A:471:TRP:CZ2	4:A:1499:GOL:H12	2.57	0.40
1:B:401:PHE:CE2	1:B:407:ALA:HB2	2.56	0.40
1:C:438:GLU:HG2	4:D:1502:GOL:C3	2.52	0.40
1:D:378:THR:HG22	1:D:398:VAL:HB	2.02	0.40
3:A:1498:NAD:H8A	3:A:1498:NAD:H2B	1.97	0.40
1:B:131:ALA:HA	1:B:132:PRO:HD3	1.88	0.40
1:C:168:LYS:C	1:C:171:PRO:HD2	2.42	0.40
1:C:429:ARG:O	1:C:433:ILE:HG12	2.21	0.40
1:D:130:LYS:HA	1:D:143:HIS:CD2	2.56	0.40
1:D:280:ILE:HD11	1:D:311:LEU:HD12	2.03	0.40
1:C:95:ILE:HG22	1:C:324:PHE:HZ	1.84	0.40
1:C:343:MET:O	1:C:346:ILE:HB	2.22	0.40
1:D:285:TRP:C	1:D:287:ASN:N	2.74	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	497/496 (100%)	456 (92%)	31 (6%)	10 (2%)	7	6
1	B	498/496 (100%)	463 (93%)	26 (5%)	9 (2%)	8	7
1	C	499/496 (101%)	458 (92%)	30 (6%)	11 (2%)	6	5
1	D	497/496 (100%)	450 (90%)	35 (7%)	12 (2%)	6	4
All	All	1991/1984 (100%)	1827 (92%)	122 (6%)	42 (2%)	7	5

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	306	GLU
1	A	358	TYR
1	A	448	GLN
1	B	306	GLU
1	B	358	TYR
1	B	448	GLN
1	C	306	GLU
1	C	358	TYR
1	C	448	GLN
1	D	306	GLU
1	D	358	TYR
1	D	364	GLU
1	D	448	GLN
1	B	187	ALA
1	B	302	SER
1	C	187	ALA
1	D	137	MET
1	D	187	ALA
1	A	4	PRO
1	A	5	ILE
1	A	187	ALA
1	B	357	LEU
1	D	357	LEU
1	B	424	SER
1	C	357	LEU
1	A	136	PRO
1	A	357	LEU
1	B	136	PRO
1	C	6	PRO

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Mol	Chain	Res	Type
1	C	302	SER
1	C	424	SER
1	D	5	ILE
1	D	6	PRO
1	D	424	SER
1	A	424	SER
1	D	363	PRO
1	C	136	PRO
1	C	272	ILE
1	D	136	PRO
1	C	417	GLY
1	B	417	GLY

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	413/409 (101%)	362 (88%)	51 (12%)	4	5
1	B	414/409 (101%)	359 (87%)	55 (13%)	4	4
1	C	415/409 (102%)	361 (87%)	54 (13%)	4	4
1	D	413/409 (101%)	357 (86%)	56 (14%)	3	3
All	All	1655/1636 (101%)	1439 (87%)	216 (13%)	4	4

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	5	ILE
1	A	8	ARG
1	A	17	ARG
1	A	27	VAL
1	A	35	ILE
1	A	48	GLU
1	A	49	VAL
1	A	59	ARG

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Mol	Chain	Res	Type
1	A	76	ARG
1	A	81	LYS
1	A	85	LYS
1	A	90	VAL
1	A	95	ILE
1	A	106	LEU
1	A	111	VAL
1	A	125	LEU
1	A	133	VAL
1	A	166	THR
1	A	181	LEU
1	A	182	LYS
1	A	189	VAL
1	A	193	GLU
1	A	196	GLU
1	A	203	LEU
1	A	222	LEU
1	A	243	VAL
1	A	254	VAL
1	A	272	ILE
1	A	275	VAL
1	A	280	ILE
1	A	294	THR
1	A	297	LEU
1	A	303	ILE
1	A	315	THR
1	A	316	LYS
1	A	320	ILE
1	A	330	LEU
1	A	348	THR
1	A	362	ARG
1	A	364	GLU
1	A	377	VAL
1	A	378	THR
1	A	384	MET
1	A	388	LYS
1	A	389	GLU
1	A	392	PHE
1	A	405	ASP
1	A	439	VAL
1	A	461	ARG
1	A	478	ASN

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Mol	Chain	Res	Type
1	B	3	PHE
1	B	5	ILE
1	B	8	ARG
1	B	17	ARG
1	B	24	ARG
1	B	27	VAL
1	B	34	GLU
1	B	35	ILE
1	B	48	GLU
1	B	49	VAL
1	B	76	ARG
1	B	81	LYS
1	B	90	VAL
1	B	91	LYS
1	B	95	ILE
1	B	106	LEU
1	B	111	VAL
1	B	125	LEU
1	B	132	PRO
1	B	133	VAL
1	B	166	THR
1	B	181	LEU
1	B	182	LYS
1	B	189	VAL
1	B	193	GLU
1	B	222	LEU
1	B	230	LYS
1	B	243	VAL
1	B	254	VAL
1	B	272	ILE
1	B	274	LYS
1	B	275	VAL
1	B	279	THR
1	B	280	ILE
1	B	294	THR
1	B	297	LEU
1	B	302	SER
1	B	303	ILE
1	B	309	ASP
1	B	315	THR
1	B	320	ILE
1	B	330	LEU

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Mol	Chain	Res	Type
1	B	348	THR
1	B	362	ARG
1	B	367	LYS
1	B	376	ILE
1	B	377	VAL
1	B	378	THR
1	B	389	GLU
1	B	392	PHE
1	B	405	ASP
1	B	439	VAL
1	B	461	ARG
1	B	478	ASN
1	B	496	SER
1	C	3	PHE
1	C	5	ILE
1	C	13	ASP
1	C	17	ARG
1	C	27	VAL
1	C	35	ILE
1	C	48	GLU
1	C	49	VAL
1	C	76	ARG
1	C	81	LYS
1	C	90	VAL
1	C	95	ILE
1	C	106	LEU
1	C	111	VAL
1	C	125	LEU
1	C	132	PRO
1	C	133	VAL
1	C	166	THR
1	C	181	LEU
1	C	182	LYS
1	C	189	VAL
1	C	193	GLU
1	C	203	LEU
1	C	222	LEU
1	C	230	LYS
1	C	243	VAL
1	C	265	VAL
1	C	271	ASP
1	C	272	ILE

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Mol	Chain	Res	Type
1	C	275	VAL
1	C	280	ILE
1	C	285	TRP
1	C	294	THR
1	C	297	LEU
1	C	302	SER
1	C	303	ILE
1	C	315	THR
1	C	316	LYS
1	C	320	ILE
1	C	326	GLU
1	C	330	LEU
1	C	348	THR
1	C	362	ARG
1	C	367	LYS
1	C	377	VAL
1	C	378	THR
1	C	384	MET
1	C	389	GLU
1	C	392	PHE
1	C	432	ARG
1	C	439	VAL
1	C	461	ARG
1	C	478	ASN
1	C	496	SER
1	D	3	PHE
1	D	5	ILE
1	D	8	ARG
1	D	17	ARG
1	D	27	VAL
1	D	35	ILE
1	D	36	ILE
1	D	48	GLU
1	D	49	VAL
1	D	76	ARG
1	D	81	LYS
1	D	86	LYS
1	D	90	VAL
1	D	95	ILE
1	D	99	LYS
1	D	106	LEU
1	D	111	VAL

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Mol	Chain	Res	Type
1	D	125	LEU
1	D	133	VAL
1	D	137	MET
1	D	141	LYS
1	D	166	THR
1	D	181	LEU
1	D	182	LYS
1	D	189	VAL
1	D	193	GLU
1	D	203	LEU
1	D	222	LEU
1	D	243	VAL
1	D	254	VAL
1	D	272	ILE
1	D	274	LYS
1	D	275	VAL
1	D	280	ILE
1	D	285	TRP
1	D	294	THR
1	D	297	LEU
1	D	303	ILE
1	D	315	THR
1	D	320	ILE
1	D	330	LEU
1	D	343	MET
1	D	348	THR
1	D	362	ARG
1	D	364	GLU
1	D	365	HIS
1	D	367	LYS
1	D	377	VAL
1	D	378	THR
1	D	384	MET
1	D	389	GLU
1	D	392	PHE
1	D	439	VAL
1	D	461	ARG
1	D	478	ASN
1	D	483	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	143	HIS
1	A	225	HIS
1	A	289	GLN
1	A	365	HIS
1	A	385	GLN
1	A	412	ASN
1	A	475	ASN
1	A	478	ASN
1	A	481	GLN
1	A	484	GLN
1	B	70	HIS
1	B	225	HIS
1	B	249	GLN
1	B	289	GLN
1	B	317	ASN
1	B	365	HIS
1	B	385	GLN
1	B	412	ASN
1	B	478	ASN
1	B	481	GLN
1	B	484	GLN
1	C	70	HIS
1	C	143	HIS
1	C	225	HIS
1	C	289	GLN
1	C	317	ASN
1	C	365	HIS
1	C	385	GLN
1	C	412	ASN
1	C	475	ASN
1	C	478	ASN
1	C	481	GLN
1	C	484	GLN
1	D	61	ASN
1	D	70	HIS
1	D	143	HIS
1	D	225	HIS
1	D	289	GLN
1	D	365	HIS
1	D	385	GLN
1	D	412	ASN
1	D	478	ASN

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Mol	Chain	Res	Type
1	D	481	GLN
1	D	484	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)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAD	B	1498	-	42,48,48	1.39	8 (19%)	50,73,73	1.57	7 (14%)
3	NAD	C	1498	-	42,48,48	1.31	5 (11%)	50,73,73	1.40	8 (16%)
4	GOL	D	1500	-	5,5,5	0.56	0	5,5,5	1.75	2 (40%)
4	GOL	A	1499	-	5,5,5	0.95	0	5,5,5	1.04	0
4	GOL	D	1499	-	5,5,5	0.74	0	5,5,5	1.46	0
4	GOL	C	1499	-	5,5,5	0.45	0	5,5,5	0.23	0
4	GOL	D	1502	-	5,5,5	0.65	0	5,5,5	0.79	0
4	GOL	A	1500	-	5,5,5	0.60	0	5,5,5	1.06	0
4	GOL	D	1501	-	5,5,5	0.43	0	5,5,5	0.80	0
3	NAD	A	1498	-	42,48,48	1.23	4 (9%)	50,73,73	1.64	9 (18%)
3	NAD	D	1498	-	42,48,48	1.26	3 (7%)	50,73,73	1.50	6 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	B	1498	-	-	2/26/62/62	0/5/5/5
3	NAD	C	1498	-	-	4/26/62/62	0/5/5/5
4	GOL	D	1500	-	-	2/4/4/4	-
4	GOL	A	1499	-	-	3/4/4/4	-
4	GOL	D	1499	-	-	4/4/4/4	-
4	GOL	C	1499	-	-	2/4/4/4	-
4	GOL	D	1502	-	-	2/4/4/4	-
4	GOL	A	1500	-	-	3/4/4/4	-
4	GOL	D	1501	-	-	2/4/4/4	-
3	NAD	A	1498	-	-	3/26/62/62	0/5/5/5
3	NAD	D	1498	-	-	5/26/62/62	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1498	NAD	C2N-N1N	-3.69	1.30	1.35
3	D	1498	NAD	O7N-C7N	3.45	1.30	1.24
3	D	1498	NAD	C2N-N1N	-3.39	1.31	1.35
3	A	1498	NAD	O7N-C7N	3.14	1.30	1.24
3	C	1498	NAD	O7N-C7N	3.09	1.29	1.24
3	C	1498	NAD	C2A-N1A	-2.59	1.29	1.33
3	A	1498	NAD	C4A-N3A	-2.48	1.32	1.35
3	C	1498	NAD	C2N-N1N	-2.48	1.32	1.35
3	A	1498	NAD	C5A-N7A	-2.42	1.31	1.39
3	C	1498	NAD	C4A-N3A	-2.39	1.32	1.35
3	B	1498	NAD	C7N-N7N	-2.36	1.28	1.33
3	B	1498	NAD	PA-O2A	-2.35	1.44	1.55
3	D	1498	NAD	PA-O2A	-2.30	1.44	1.55
3	B	1498	NAD	O7N-C7N	2.22	1.28	1.24
3	A	1498	NAD	PA-O2A	-2.22	1.45	1.55
3	B	1498	NAD	C5A-N7A	-2.20	1.31	1.39
3	B	1498	NAD	C3N-C7N	-2.06	1.47	1.50
3	B	1498	NAD	O4B-C4B	-2.06	1.40	1.45
3	C	1498	NAD	C5A-N7A	-2.02	1.32	1.39
3	B	1498	NAD	C6N-N1N	-2.01	1.30	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1498	NAD	N3A-C2A-N1A	-6.26	120.17	128.67
3	B	1498	NAD	N3A-C2A-N1A	-5.76	120.85	128.67
3	C	1498	NAD	N3A-C2A-N1A	-5.43	121.31	128.67
3	A	1498	NAD	C4B-O4B-C1B	4.88	114.39	109.92
3	A	1498	NAD	N3A-C2A-N1A	-4.57	122.47	128.67
3	B	1498	NAD	O7N-C7N-N7N	-4.03	116.79	122.62
3	B	1498	NAD	O4B-C1B-N9A	-3.60	103.97	108.75
3	B	1498	NAD	C3N-C7N-N7N	3.37	121.89	117.74
3	C	1498	NAD	C4A-C5A-N7A	-3.33	105.81	109.34
3	A	1498	NAD	O7N-C7N-N7N	-3.24	117.93	122.62
3	A	1498	NAD	C5N-C4N-C3N	-3.18	117.24	120.36
3	B	1498	NAD	C5N-C4N-C3N	-3.06	117.36	120.36
3	A	1498	NAD	O2B-C2B-C3B	-3.05	102.04	111.82
3	D	1498	NAD	C3N-C7N-N7N	3.02	121.47	117.74
3	A	1498	NAD	O2N-PN-O3	2.96	115.27	107.27
3	C	1498	NAD	O7N-C7N-N7N	-2.95	118.35	122.62
3	B	1498	NAD	C5D-C4D-C3D	-2.78	105.21	115.21
3	A	1498	NAD	O2A-PA-O3	2.76	114.73	107.27
3	D	1498	NAD	O2N-PN-O3	2.59	114.26	107.27
3	D	1498	NAD	C5N-C4N-C3N	-2.58	117.83	120.36
3	C	1498	NAD	O2A-PA-O3	2.51	114.06	107.27
3	C	1498	NAD	C5N-C4N-C3N	-2.41	117.99	120.36
3	A	1498	NAD	C6N-N1N-C2N	-2.38	119.85	121.88
4	D	1500	GOL	O1-C1-C2	2.27	120.58	110.38
3	D	1498	NAD	C4A-C5A-N7A	-2.26	106.95	109.34
3	C	1498	NAD	O3-PA-O1A	-2.24	103.96	110.70
3	B	1498	NAD	C4A-C5A-N7A	-2.22	106.99	109.34
3	C	1498	NAD	C3N-C7N-N7N	2.16	120.40	117.74
3	A	1498	NAD	O7N-C7N-C3N	2.13	122.20	119.60
3	C	1498	NAD	C5A-C6A-N6A	2.02	123.39	120.31
3	D	1498	NAD	C6N-N1N-C2N	-2.02	120.16	121.88
4	D	1500	GOL	O2-C2-C1	2.02	117.55	109.18

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1498	NAD	C5B-O5B-PA-O1A
3	D	1498	NAD	C5B-O5B-PA-O2A
3	D	1498	NAD	C5B-O5B-PA-O3
4	A	1499	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	1500	GOL	O1-C1-C2-C3
4	D	1499	GOL	C1-C2-C3-O3
4	D	1500	GOL	O1-C1-C2-O2
4	D	1501	GOL	C1-C2-C3-O3
4	D	1502	GOL	C1-C2-C3-O3
4	A	1499	GOL	O1-C1-C2-O2
4	C	1499	GOL	O2-C2-C3-O3
4	C	1499	GOL	C1-C2-C3-O3
4	D	1499	GOL	O1-C1-C2-C3
4	D	1500	GOL	O1-C1-C2-C3
3	A	1498	NAD	C3D-C4D-C5D-O5D
4	A	1500	GOL	O1-C1-C2-O2
4	D	1499	GOL	O2-C2-C3-O3
4	D	1502	GOL	O2-C2-C3-O3
4	A	1500	GOL	C1-C2-C3-O3
3	D	1498	NAD	O4B-C4B-C5B-O5B
3	A	1498	NAD	O4D-C4D-C5D-O5D
3	B	1498	NAD	PN-O3-PA-O5B
4	D	1501	GOL	O2-C2-C3-O3
3	C	1498	NAD	C5B-O5B-PA-O1A
3	C	1498	NAD	C5B-O5B-PA-O2A
3	C	1498	NAD	C5B-O5B-PA-O3
3	D	1498	NAD	C5B-O5B-PA-O1A
3	C	1498	NAD	C4D-C5D-O5D-PN
3	B	1498	NAD	C4D-C5D-O5D-PN
4	D	1499	GOL	O1-C1-C2-O2
3	D	1498	NAD	C4D-C5D-O5D-PN
4	A	1499	GOL	O2-C2-C3-O3

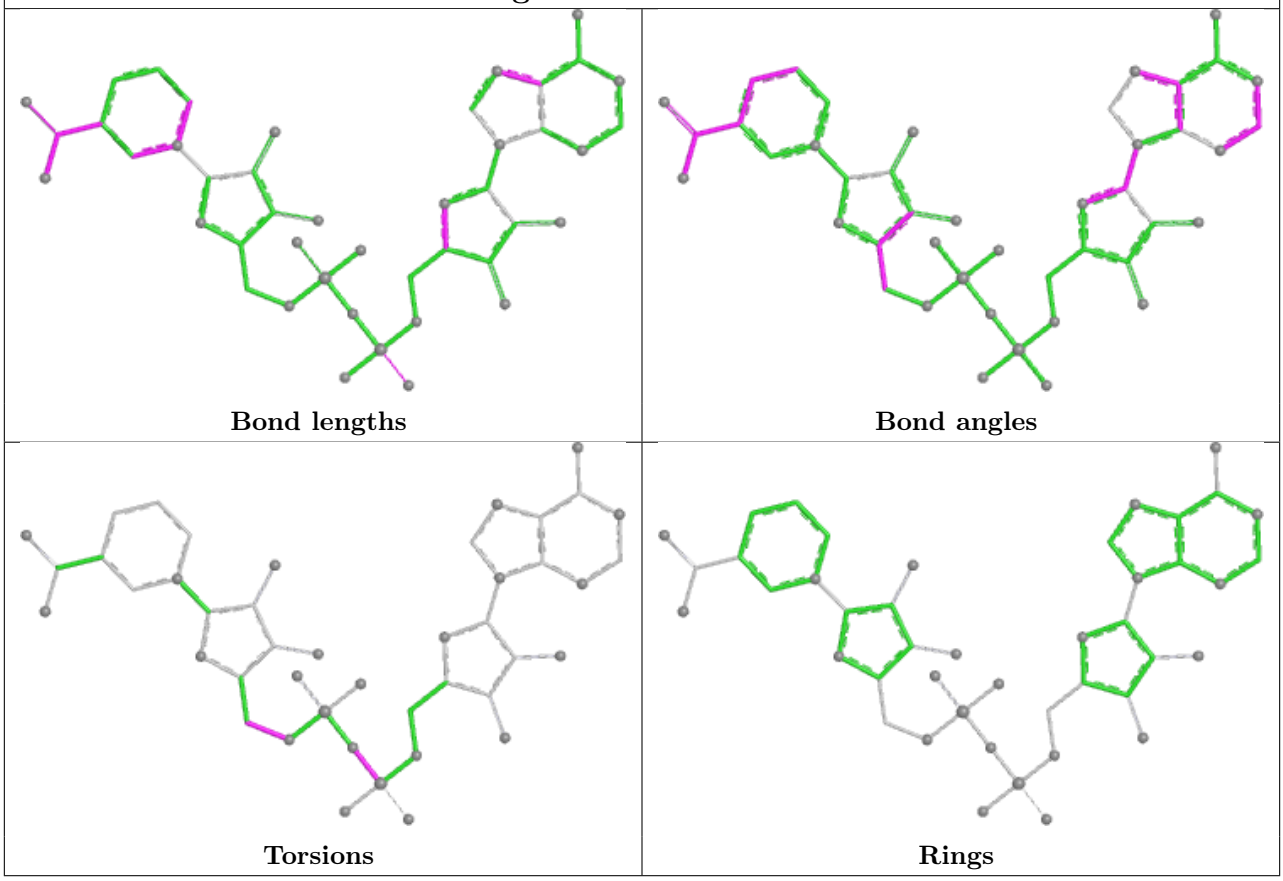
There are no ring outliers.

9 monomers are involved in 46 short contacts:

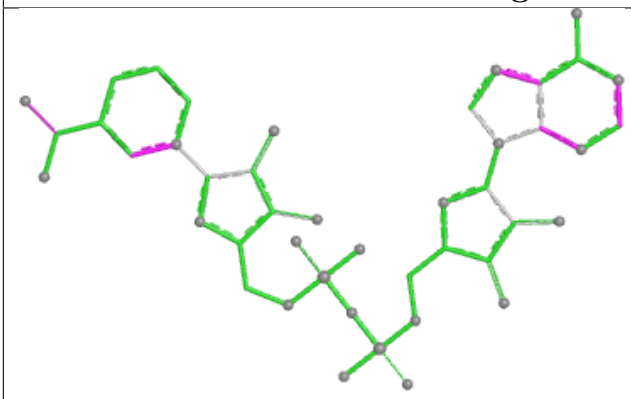
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1498	NAD	9	0
3	C	1498	NAD	8	0
4	D	1500	GOL	4	0
4	A	1499	GOL	1	0
4	C	1499	GOL	8	0
4	D	1502	GOL	2	0
4	D	1501	GOL	3	0
3	A	1498	NAD	5	0
3	D	1498	NAD	6	0

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

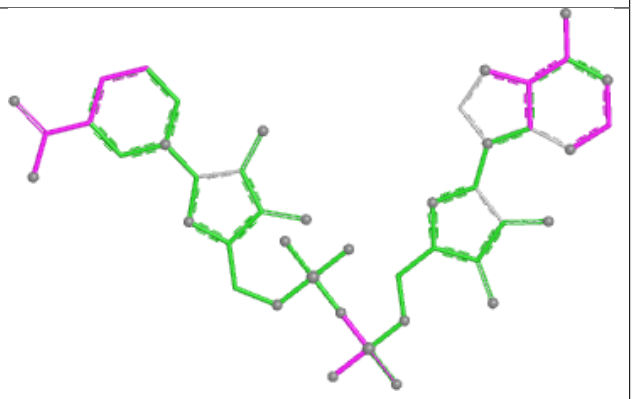
Ligand NAD B 1498



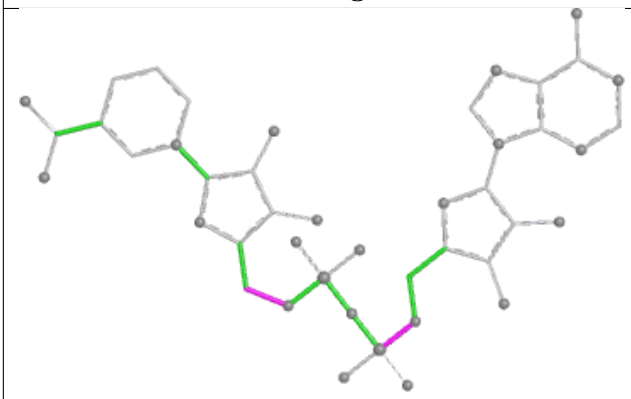
Ligand NAD C 1498



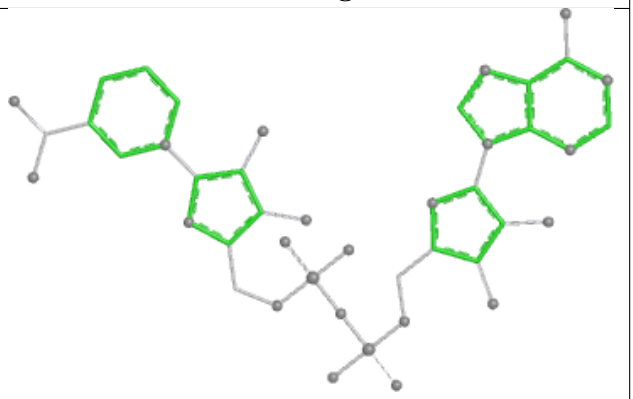
Bond lengths



Bond angles

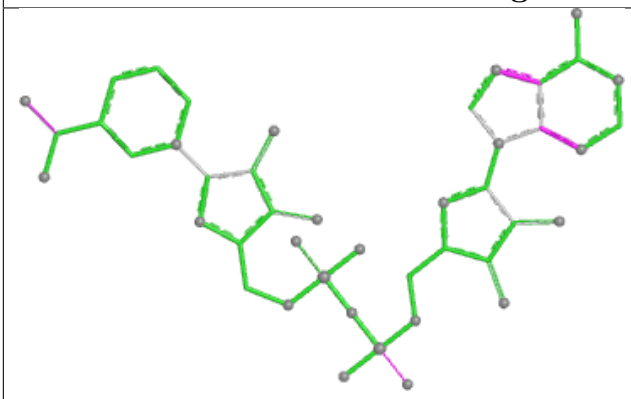


Torsions

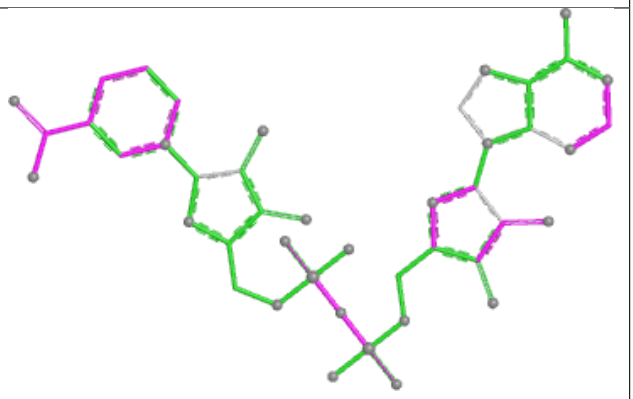


Rings

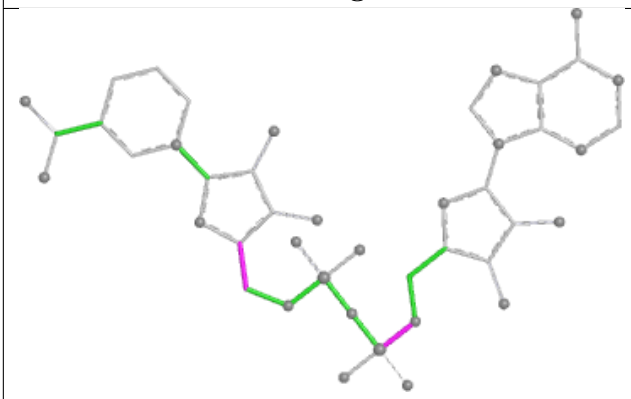
Ligand NAD A 1498



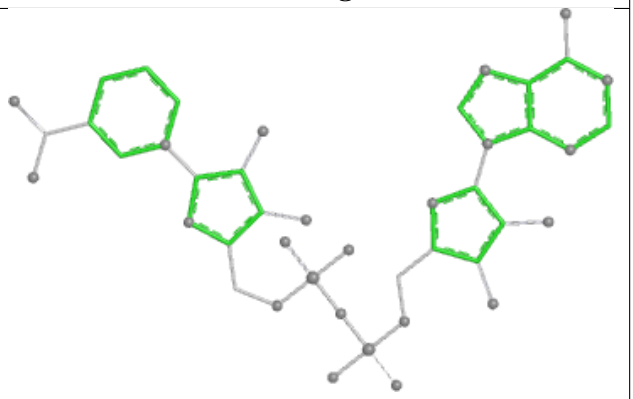
Bond lengths



Bond angles

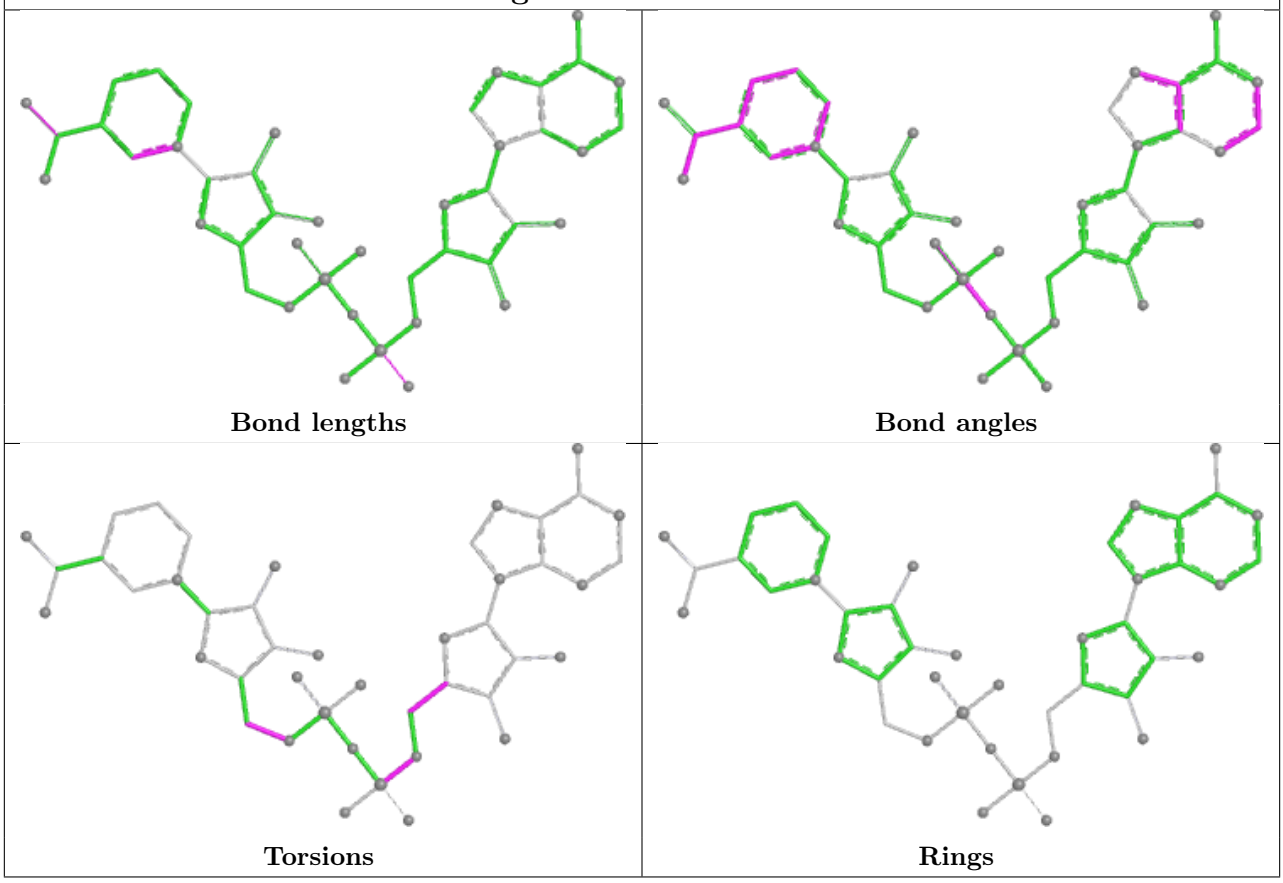


Torsions



Rings

Ligand NAD D 1498



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

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	494/496 (99%)	0.47	25 (5%)	28 35	26, 52, 74, 103	0
1	B	494/496 (99%)	0.57	40 (8%)	12 16	24, 52, 74, 111	0
1	C	494/496 (99%)	0.65	40 (8%)	12 16	26, 57, 81, 93	0
1	D	494/496 (99%)	0.76	54 (10%)	5 8	29, 58, 84, 95	0
All	All	1976/1984 (99%)	0.61	159 (8%)	12 16	24, 54, 80, 111	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	402	SER	6.0
1	D	3	PHE	5.6
1	B	3	PHE	5.4
1	D	61	ASN	5.2
1	A	61	ASN	5.2
1	C	305	ALA	4.8
1	B	324	PHE	4.7
1	A	327	GLY	4.2
1	C	80	ALA	4.2
1	C	73	THR	4.1
1	C	15	GLU	3.9
1	D	313	LYS	3.9
1	D	95	ILE	3.8
1	A	325	GLU	3.7
1	D	288	GLY	3.6
1	D	181	LEU	3.6
1	C	14	GLY	3.5
1	D	336	LYS	3.4
1	A	487	SER	3.4
1	C	61	ASN	3.3
1	C	367	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	425	ASN	3.2
1	D	409	ALA	3.2
1	B	428	GLU	3.2
1	C	4	PRO	3.2
1	A	95	ILE	3.2
1	B	102	ASP	3.2
1	B	367	LYS	3.2
1	D	284	PHE	3.1
1	D	496	SER	3.1
1	B	22	LYS	3.1
1	C	181	LEU	3.1
1	D	339	TYR	3.1
1	D	373	GLU	3.1
1	B	316	LYS	3.0
1	C	3	PHE	3.0
1	B	283	CYS	3.0
1	C	191	CYS	3.0
1	A	154	LEU	3.0
1	A	488	ASP	3.0
1	B	326	GLU	3.0
1	C	119	ALA	3.0
1	C	310	LYS	2.9
1	B	32	THR	2.9
1	A	282	GLY	2.9
1	A	284	PHE	2.8
1	D	317	ASN	2.8
1	C	6	PRO	2.8
1	D	293	ALA	2.8
1	C	183	PRO	2.8
1	B	343	MET	2.8
1	C	101	PHE	2.7
1	D	427	LEU	2.7
1	A	326	GLU	2.7
1	D	280	ILE	2.7
1	D	267	PHE	2.7
1	D	28	ILE	2.7
1	A	283	CYS	2.7
1	D	380	ILE	2.7
1	B	309	ASP	2.7
1	D	353	GLY	2.7
1	B	368	LYS	2.7
1	D	279	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	164	MET	2.6
1	D	383[A]	SER	2.6
1	D	98	GLY	2.6
1	C	122	ALA	2.6
1	D	282	GLY	2.6
1	B	87	ASP	2.6
1	C	328	CYS	2.6
1	D	283	CYS	2.6
1	A	79	ALA	2.6
1	B	369	GLY	2.6
1	A	210	ILE	2.6
1	C	210	ILE	2.6
1	D	294	THR	2.5
1	B	327	GLY	2.5
1	C	105	VAL	2.5
1	D	188	SER	2.5
1	D	396	LEU	2.5
1	C	123	GLU	2.5
1	D	384	MET	2.5
1	D	359	GLY	2.5
1	D	208	LEU	2.5
1	A	164	MET	2.5
1	C	154	LEU	2.5
1	C	59	ARG	2.4
1	B	421	ALA	2.4
1	D	180	VAL	2.4
1	C	155	ILE	2.4
1	D	133	VAL	2.4
1	D	365	HIS	2.4
1	D	31	SER	2.4
1	D	421	ALA	2.4
1	A	22	LYS	2.4
1	D	210	ILE	2.4
1	B	20	ILE	2.4
1	D	272	ILE	2.4
1	B	7	ALA	2.4
1	B	165	ALA	2.4
1	B	364	GLU	2.4
1	C	34	GLU	2.4
1	B	95	ILE	2.3
1	B	18	GLU	2.3
1	A	18	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	181	LEU	2.3
1	A	288	GLY	2.3
1	B	365	HIS	2.3
1	C	496	SER	2.3
1	D	105	VAL	2.3
1	D	303	ILE	2.3
1	B	282	GLY	2.3
1	A	280	ILE	2.3
1	C	394	PRO	2.3
1	D	369	GLY	2.2
1	D	492	GLY	2.2
1	B	191	CYS	2.2
1	B	388	LYS	2.2
1	A	383[A]	SER	2.2
1	B	496	SER	2.2
1	C	486	ILE	2.2
1	C	187	ALA	2.2
1	D	410	LEU	2.2
1	B	187	ALA	2.2
1	B	279	THR	2.2
1	C	165	ALA	2.2
1	A	492	GLY	2.2
1	D	211	LEU	2.2
1	C	127	GLY	2.2
1	A	3	PHE	2.2
1	C	95	ILE	2.2
1	A	162	LEU	2.2
1	B	183	PRO	2.2
1	D	490	PRO	2.2
1	C	327	GLY	2.1
1	A	174	ALA	2.1
1	B	447	SER	2.1
1	D	183	PRO	2.1
1	D	491	TRP	2.1
1	C	354	ALA	2.1
1	D	368	LYS	2.1
1	B	303	ILE	2.1
1	C	168	LYS	2.1
1	D	191	CYS	2.1
1	D	367	LYS	2.1
1	D	285	TRP	2.1
1	C	190	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	330	LEU	2.1
1	C	184	SER	2.1
1	B	36	ILE	2.1
1	C	162	LEU	2.0
1	B	431	GLU	2.0
1	D	326	GLU	2.0
1	B	101	PHE	2.0
1	B	23	ASN	2.0
1	B	297	LEU	2.0
1	A	369	GLY	2.0
1	B	91	LYS	2.0
1	B	321	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, 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	K	D	1497	1/1	0.70	0.22	94,94,94,94	0
4	GOL	D	1501	6/6	0.75	0.19	58,61,64,73	0
4	GOL	D	1502	6/6	0.79	0.26	62,65,73,74	0
2	K	C	1501	1/1	0.81	0.16	64,64,64,64	0
2	K	A	1497	1/1	0.84	0.14	85,85,85,85	0
4	GOL	D	1500	6/6	0.85	0.27	41,51,52,65	0
4	GOL	A	1500	6/6	0.85	0.20	51,59,65,65	0
4	GOL	D	1499	6/6	0.85	0.23	45,50,54,58	0
4	GOL	C	1499	6/6	0.86	0.34	54,62,64,73	0
2	K	B	1499	1/1	0.88	0.21	69,69,69,69	0
2	K	C	1497	1/1	0.90	0.11	85,85,85,85	0

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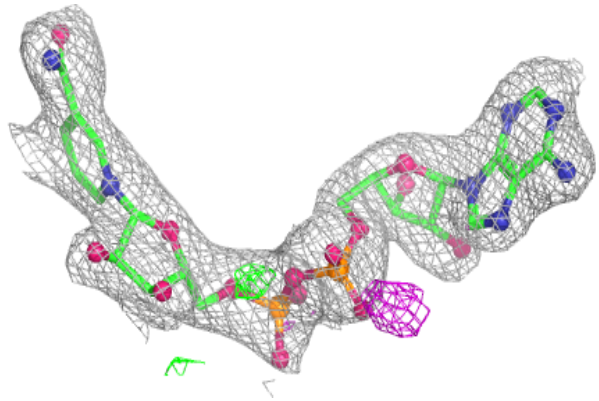
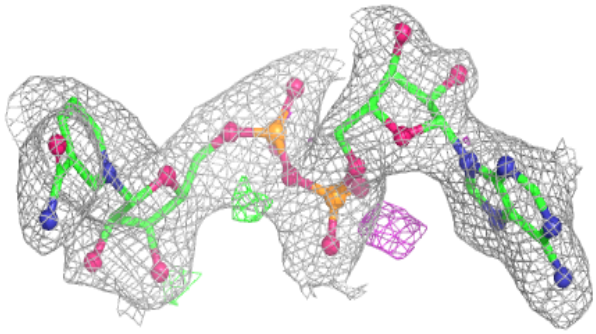
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	1499	6/6	0.91	0.16	56,61,69,70	0
3	NAD	D	1498	44/44	0.92	0.14	38,51,61,70	0
3	NAD	A	1498	44/44	0.92	0.13	34,48,58,71	0
2	K	A	1501	1/1	0.93	0.29	76,76,76,76	0
3	NAD	C	1498	44/44	0.93	0.14	37,49,62,66	0
2	K	C	1500	1/1	0.94	0.19	69,69,69,69	0
3	NAD	B	1498	44/44	0.96	0.11	31,43,51,55	0
2	K	B	1497	1/1	0.96	0.09	63,63,63,63	0

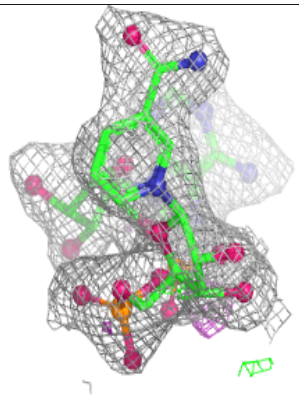
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 1498:

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

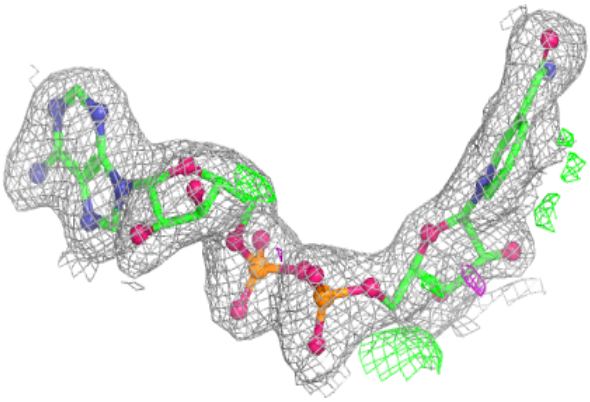


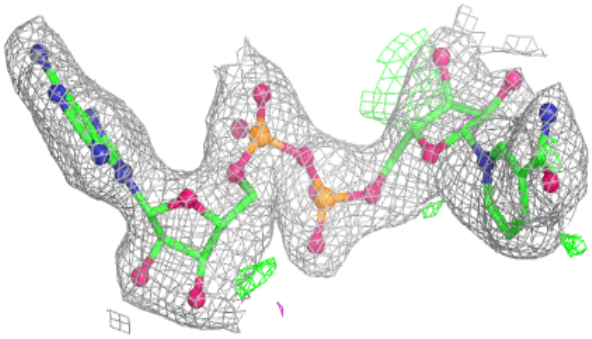


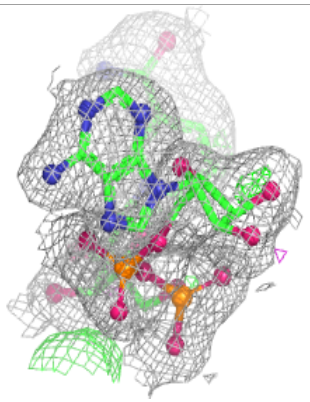


Electron density around NAD A 1498:

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

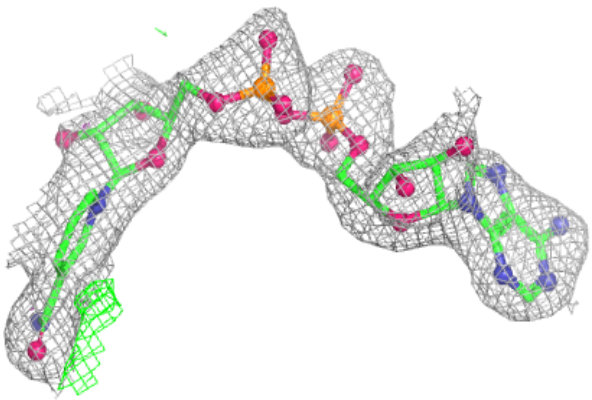


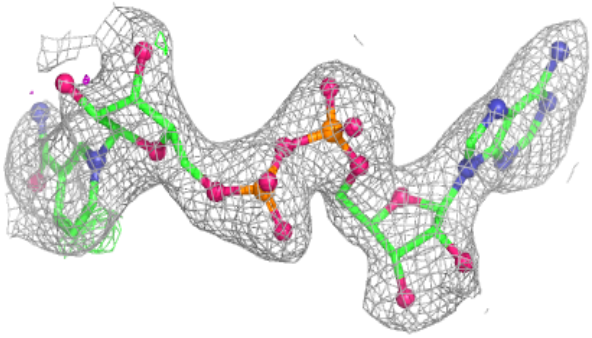


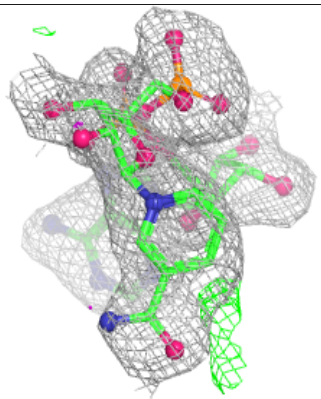


Electron density around NAD C 1498:

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

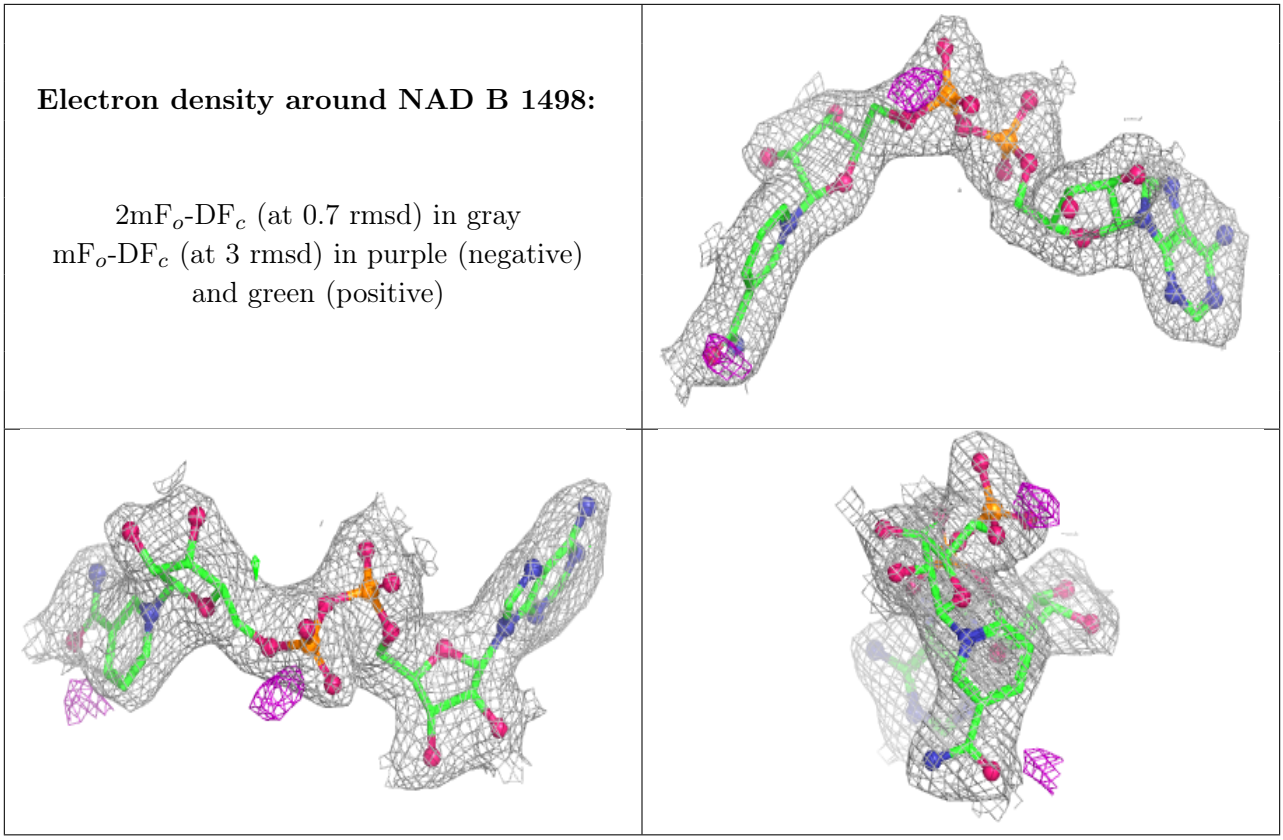






Electron density around NAD B 1498:

$2mF_o$-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.