



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:19 AM UTC

PDB ID : 1HZZ / pdb_00001hzz
Title : THE ASYMMETRIC COMPLEX OF THE TWO NUCLEOTIDE-BINDING COMPONENTS (DI, DIII) OF PROTON-TRANSLOCATING TRANSHYDROGENASE
Authors : Cotton, N.P.J.; White, S.A.; Peake, S.J.; McSweeney, S.; Jackson, J.B.
Deposited on : 2001-01-27
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

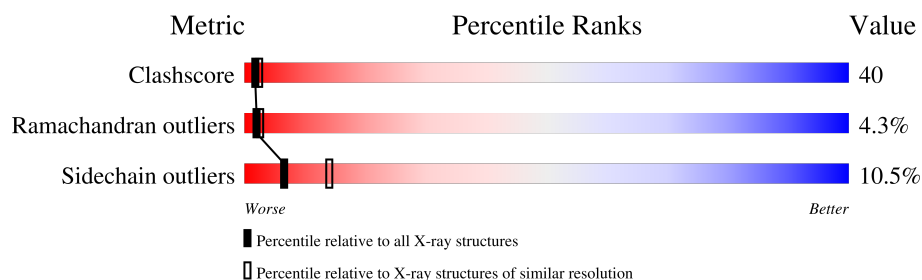
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	384	
1	B	384	
2	C	203	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6835 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.

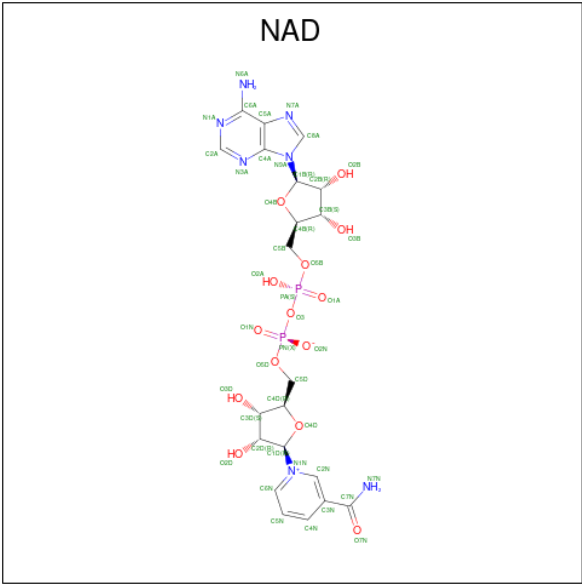
- Molecule 1 is a protein called PROTON-TRANSLCATING NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT PNTAA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2666	1684	460	505	17			
1	B	366	Total	C	N	O	S	0	0	0
			2692	1701	465	509	17			

- Molecule 2 is a protein called PROTON-TRANSLCATING NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT PNTB.

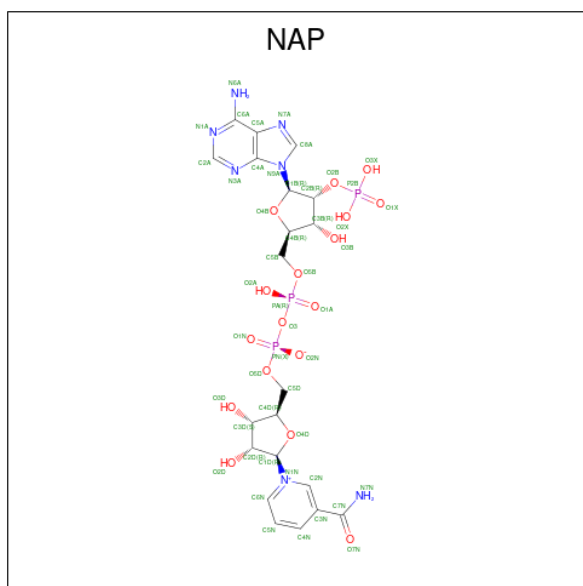
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	174	Total	C	N	O	S	0	0	0
			1311	830	217	253	11			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is water.

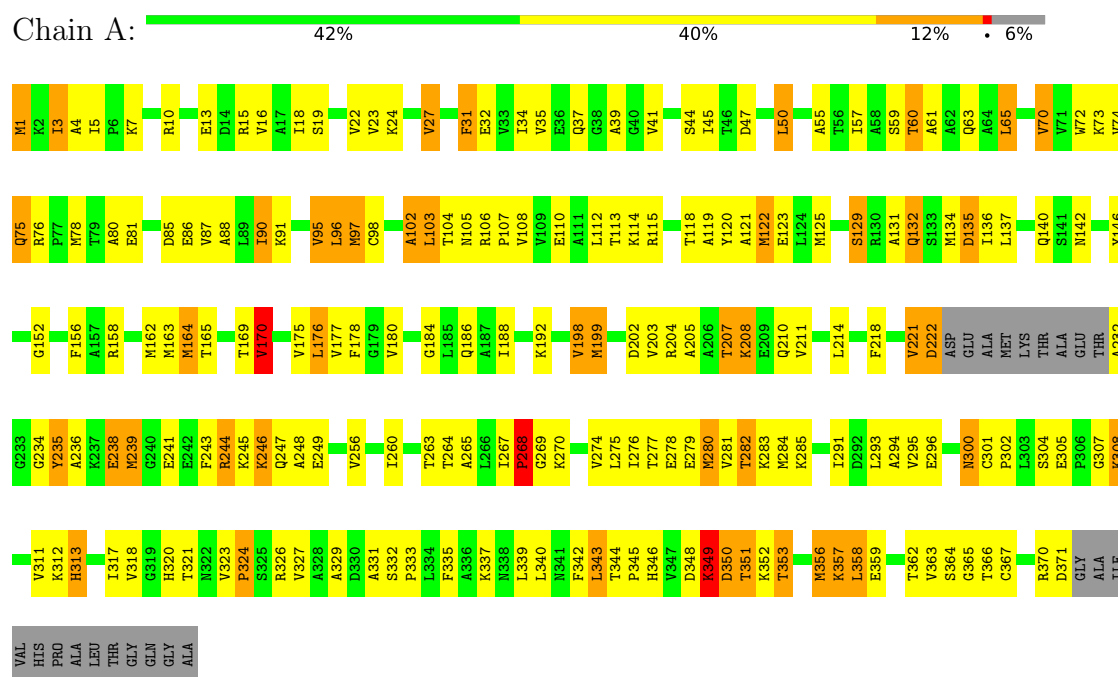
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	40	Total	O	0	0
			40	40		
5	C	9	Total	O	0	0
			9	9		

3 Residue-property plots

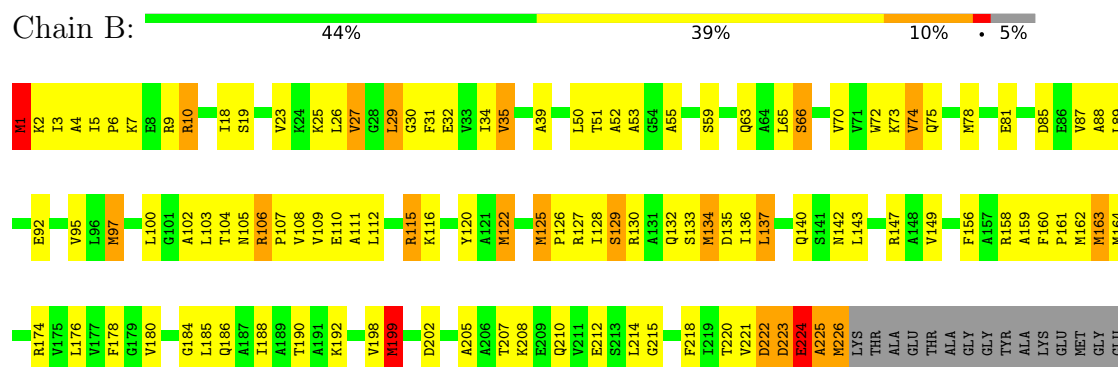
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

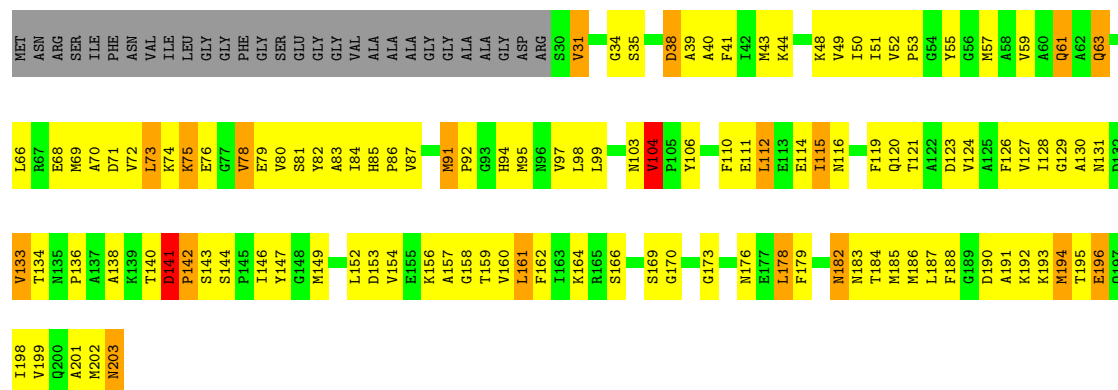
Note EDS was not executed.

• Molecule 1: PROTON-TRANSLOCATING NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT PNTAA



• Molecule 1: PROTON-TRANSLOCATING NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT PNTAA





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.48Å 74.17Å 205.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.96 – 2.50	Depositor
% Data completeness (in resolution range)	95.0 (24.96-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6835	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.82	24/2700 (0.9%)	1.03	16/3656 (0.4%)
1	B	1.05	34/2727 (1.2%)	1.19	17/3697 (0.5%)
2	C	0.79	2/1334 (0.1%)	1.09	10/1803 (0.6%)
All	All	0.91	60/6761 (0.9%)	1.11	43/9156 (0.5%)

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	GLY	C-O	20.64	1.64	1.23
2	C	203	ASN	C-OXT	20.13	1.63	1.23
1	B	226	MET	SD-CE	12.13	2.09	1.79
1	B	348	ASP	C-N	11.97	1.50	1.33
1	B	226	MET	CG-SD	11.69	2.10	1.80
1	A	222	ASP	C-O	10.01	1.43	1.23
1	A	239	MET	SD-CE	9.45	2.03	1.79
1	A	239	MET	CG-SD	8.77	2.02	1.80
1	B	223	ASP	C-O	8.69	1.34	1.24
1	B	224	GLU	C-O	7.84	1.33	1.24
1	B	350	ASP	CA-C	-7.41	1.42	1.52
1	A	1	MET	SD-CE	7.19	1.97	1.79
1	B	1	MET	SD-CE	6.91	1.96	1.79
1	A	199	MET	SD-CE	6.86	1.96	1.79
1	B	1	MET	CG-SD	6.64	1.97	1.80
1	B	199	MET	SD-CE	6.56	1.96	1.79
1	A	280	MET	CG-SD	6.45	1.96	1.80
1	A	284	MET	CG-SD	6.40	1.96	1.80
1	A	164	MET	SD-CE	6.35	1.95	1.79
1	A	78	MET	SD-CE	6.33	1.95	1.79
1	B	164	MET	SD-CE	6.33	1.95	1.79
2	C	203	ASN	C-O	6.30	1.36	1.23
1	A	162	MET	SD-CE	6.25	1.95	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	MET	CG-SD	6.24	1.96	1.80
1	B	163	MET	SD-CE	6.24	1.95	1.79
1	B	162	MET	SD-CE	6.23	1.95	1.79
1	A	78	MET	CG-SD	6.17	1.96	1.80
1	A	125	MET	CG-SD	6.12	1.96	1.80
1	A	1	MET	CG-SD	6.11	1.96	1.80
1	A	125	MET	SD-CE	6.11	1.94	1.79
1	B	78	MET	SD-CE	6.08	1.94	1.79
1	B	162	MET	CG-SD	6.04	1.95	1.80
1	B	125	MET	SD-CE	6.03	1.94	1.79
1	B	356	MET	CG-SD	6.03	1.95	1.80
1	B	280	MET	SD-CE	6.02	1.94	1.79
1	B	280	MET	CG-SD	5.99	1.95	1.80
1	A	134	MET	SD-CE	5.97	1.94	1.79
1	A	356	MET	CG-SD	5.92	1.95	1.80
1	B	97	MET	SD-CE	5.90	1.94	1.79
1	B	134	MET	SD-CE	5.88	1.94	1.79
1	B	122	MET	CG-SD	5.79	1.95	1.80
1	B	284	MET	CG-SD	5.72	1.95	1.80
1	A	97	MET	SD-CE	5.71	1.93	1.79
1	B	356	MET	SD-CE	5.70	1.93	1.79
1	B	78	MET	CG-SD	5.70	1.95	1.80
1	A	162	MET	CG-SD	5.68	1.95	1.80
1	B	97	MET	CG-SD	5.63	1.94	1.80
1	A	356	MET	SD-CE	5.57	1.93	1.79
1	B	349	LYS	C-N	-5.57	1.25	1.33
1	A	280	MET	SD-CE	5.55	1.93	1.79
1	B	164	MET	CG-SD	5.50	1.94	1.80
1	A	122	MET	SD-CE	5.41	1.93	1.79
1	A	122	MET	CG-SD	5.41	1.94	1.80
1	B	199	MET	CG-SD	5.39	1.94	1.80
1	B	125	MET	CG-SD	5.38	1.94	1.80
1	B	122	MET	SD-CE	5.31	1.92	1.79
1	B	163	MET	CG-SD	5.22	1.93	1.80
1	B	284	MET	SD-CE	5.15	1.92	1.79
1	A	284	MET	SD-CE	5.14	1.92	1.79
1	B	134	MET	CG-SD	5.02	1.93	1.80

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	ASP	O-C-N	14.73	142.18	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ASP	N-CA-C	-13.15	96.95	111.28
1	B	247	GLN	N-CA-C	-9.26	99.57	112.45
2	C	73	LEU	N-CA-C	-8.99	100.72	112.68
1	B	350	ASP	N-CA-C	-8.83	91.99	110.80
1	B	226	MET	CB-CG-SD	-8.22	88.03	112.70
1	A	32	GLU	N-CA-C	-8.04	96.13	109.24
1	B	351	THR	O-C-N	7.84	133.02	122.59
1	B	244	ARG	N-CA-C	-6.63	105.25	113.15
1	A	169	THR	CA-C-N	-6.47	118.20	122.60
1	A	169	THR	C-N-CA	-6.47	118.20	122.60
1	B	250	ALA	N-CA-C	-6.22	104.04	111.69
1	A	129	SER	N-CA-C	6.16	118.96	111.82
1	B	300	ASN	N-CA-C	-6.15	105.78	113.28
1	B	350	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	41	VAL	N-CA-C	5.99	116.45	110.23
2	C	76	GLU	N-CA-C	-5.95	103.97	111.11
1	A	198	VAL	N-CA-C	5.92	117.87	108.87
1	A	208	LYS	N-CA-C	5.90	118.47	111.33
1	B	224	GLU	N-CA-C	-5.80	98.45	110.80
1	A	214	LEU	N-CA-C	-5.76	106.29	113.38
2	C	75	LYS	N-CA-C	-5.71	104.44	111.40
1	A	170	VAL	N-CA-C	-5.68	102.39	107.56
2	C	166	SER	N-CA-C	5.56	114.89	108.49
1	A	170	VAL	CA-C-N	5.53	123.64	119.66
1	A	170	VAL	C-N-CA	5.53	123.64	119.66
2	C	103	ASN	N-CA-C	5.53	119.32	112.58
1	A	27	VAL	N-CA-C	-5.51	105.13	110.42
2	C	80	VAL	N-CA-C	5.49	116.38	108.48
1	B	27	VAL	N-CA-C	-5.42	104.59	110.23
1	A	343	LEU	N-CA-C	5.40	116.97	111.14
2	C	141	ASP	CA-C-N	5.40	126.58	119.84
2	C	141	ASP	C-N-CA	5.40	126.58	119.84
1	A	205	ALA	N-CA-C	5.37	116.94	111.14
1	B	100	LEU	N-CA-C	5.36	117.21	111.36
1	B	343	LEU	N-CA-C	5.31	117.88	111.40
1	B	308	LYS	N-CA-C	5.30	117.04	109.14
1	B	350	ASP	CA-C-N	5.23	131.53	121.54
1	B	350	ASP	C-N-CA	5.23	131.53	121.54
1	A	300	ASN	N-CA-C	-5.16	106.66	113.17
2	C	104	VAL	CA-C-N	5.13	125.42	119.93
2	C	104	VAL	C-N-CA	5.13	125.42	119.93
1	A	170	VAL	CA-C-O	5.13	121.99	119.12

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	2666	0	2794	205	0
1	B	2692	0	2824	221	0
2	C	1311	0	1303	131	0
3	A	44	0	23	3	0
4	C	48	0	25	3	0
5	A	25	0	0	4	0
5	B	40	0	0	9	0
5	C	9	0	0	6	0
All	All	6835	0	6969	551	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 40.

All (551) 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:A:239:MET:SD	1:A:239:MET:CE	2.03	1.47
1:A:239:MET:SD	1:A:239:MET:CG	2.02	1.45
1:B:226:MET:CE	1:B:226:MET:SD	2.09	1.40
1:B:226:MET:SD	1:B:226:MET:CG	2.10	1.39
2:C:203:ASN:C	2:C:203:ASN:OXT	1.63	1.39
1:B:381:GLY:C	1:B:381:GLY:O	1.64	1.37
1:B:349:LYS:O	1:B:350:ASP:CG	1.86	1.18
1:B:351:THR:O	1:B:352:LYS:HG3	1.49	1.12
1:A:277:THR:H	1:A:280:MET:HE3	1.06	1.11
1:B:115:ARG:HH11	1:B:115:ARG:HB3	1.13	1.08
1:A:221:VAL:HG22	1:A:222:ASP:H	1.15	1.08
1:B:349:LYS:O	1:B:350:ASP:OD2	1.76	1.02
2:C:53:PRO:HB2	2:C:95:MET:HE2	1.40	1.01
2:C:127:VAL:HG13	2:C:130:ALA:HB3	1.43	1.00
1:B:97:MET:HB3	1:B:122:MET:HE1	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:MET:SD	1:B:226:MET:CA	2.51	0.98
1:B:174:ARG:HH21	1:B:199:MET:HE1	1.31	0.94
1:A:65:LEU:H	1:A:65:LEU:HD22	1.34	0.92
1:B:2:LYS:HE2	1:B:34:ILE:HD11	1.50	0.92
1:A:275:LEU:HD12	1:A:300:ASN:HB3	1.50	0.92
1:A:277:THR:N	1:A:280:MET:HE3	1.85	0.91
2:C:195:THR:O	2:C:199:VAL:HG23	1.72	0.90
2:C:111:GLU:HG3	2:C:114:GLU:HG2	1.54	0.89
1:B:226:MET:SD	1:B:226:MET:CB	2.60	0.89
1:B:10:ARG:HG3	1:B:10:ARG:HH11	1.40	0.87
1:A:277:THR:H	1:A:280:MET:CE	1.86	0.86
1:A:97:MET:HE1	1:A:343:LEU:HD12	1.58	0.86
1:B:224:GLU:OE1	1:B:226:MET:N	2.09	0.85
1:A:158:ARG:HG2	1:B:329:ALA:HB3	1.56	0.85
1:B:351:THR:O	1:B:352:LYS:CG	2.25	0.85
1:A:7:LYS:HG2	1:A:39:ALA:HA	1.58	0.83
1:B:351:THR:O	1:B:351:THR:HG23	1.78	0.83
2:C:69:MET:HE1	2:C:126:PHE:CD2	2.14	0.82
2:C:99:LEU:HB3	2:C:104:VAL:HG11	1.61	0.82
1:B:174:ARG:NH2	1:B:199:MET:HE1	1.93	0.82
1:B:281:VAL:HA	1:B:284:MET:HE3	1.60	0.82
1:B:226:MET:HE2	1:B:244:ARG:HH22	1.45	0.82
2:C:99:LEU:HB3	2:C:104:VAL:CG1	2.09	0.82
1:A:221:VAL:HG22	1:A:222:ASP:N	1.96	0.81
1:B:368:VAL:HG12	1:B:369:THR:HG22	1.61	0.81
1:A:87:VAL:HG13	1:A:112:LEU:HD23	1.62	0.81
1:A:207:THR:HA	1:A:210:GLN:HE21	1.44	0.81
2:C:127:VAL:CG1	2:C:130:ALA:HB3	2.12	0.79
2:C:53:PRO:HB2	2:C:95:MET:CE	2.11	0.79
1:B:226:MET:SD	1:B:226:MET:HA	2.23	0.79
2:C:39:ALA:HB2	2:C:187:LEU:HD21	1.65	0.78
1:B:255:LEU:HD21	1:B:284:MET:HE2	1.65	0.78
1:A:106:ARG:N	1:A:107:PRO:HD2	1.98	0.78
1:A:3:ILE:HG13	1:A:70:VAL:HG22	1.65	0.77
1:B:252:LEU:O	1:B:256:VAL:HG23	1.85	0.77
1:B:115:ARG:HH11	1:B:115:ARG:CB	1.94	0.76
1:B:87:VAL:HG23	1:B:112:LEU:HD23	1.68	0.76
1:B:97:MET:HE1	1:B:343:LEU:HD13	1.67	0.76
2:C:112:LEU:C	2:C:112:LEU:HD23	2.11	0.76
1:B:221:VAL:HG11	1:B:247:GLN:HA	1.69	0.75
1:B:276:ILE:HG12	5:B:402:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HB	1:A:95:VAL:HG22	1.69	0.74
2:C:66:LEU:HD13	2:C:128:ILE:HD13	1.70	0.73
1:B:25:LYS:O	1:B:29:LEU:HD12	1.87	0.73
2:C:85:HIS:CE1	2:C:87:VAL:HG22	2.23	0.73
1:B:115:ARG:HB3	1:B:115:ARG:NH1	1.96	0.73
2:C:50:ILE:HG22	2:C:81:SER:HB2	1.70	0.73
2:C:185:MET:O	2:C:186:MET:HE2	1.88	0.73
1:B:226:MET:HE2	1:B:244:ARG:NH2	2.03	0.73
1:A:329:ALA:HB3	1:B:158:ARG:HG3	1.71	0.72
1:B:226:MET:HE2	5:B:421:HOH:O	1.89	0.72
2:C:43:MET:HE1	2:C:69:MET:HE3	1.70	0.72
1:B:88:ALA:HA	1:B:115:ARG:HE	1.54	0.72
1:A:221:VAL:CG2	1:A:222:ASP:H	1.99	0.71
2:C:154:VAL:HG23	2:C:178:LEU:HD11	1.71	0.71
1:B:269:GLY:C	1:B:270:LYS:HD2	2.15	0.71
1:A:203:VAL:HB	1:A:239:MET:HE2	1.73	0.70
1:A:222:ASP:HA	1:A:246:LYS:HD2	1.71	0.70
1:B:222:ASP:OD2	1:B:225:ALA:HA	1.91	0.70
1:B:226:MET:SD	1:B:226:MET:N	2.64	0.70
1:B:284:MET:HE1	1:B:290:ILE:HD11	1.72	0.70
1:B:225:ALA:O	1:B:226:MET:C	2.34	0.70
1:B:222:ASP:CG	1:B:225:ALA:HA	2.17	0.70
1:B:178:PHE:HB3	1:B:275:LEU:HD13	1.73	0.70
2:C:116:ASN:OD1	2:C:152:LEU:HA	1.93	0.69
1:A:1:MET:H3	1:A:352:LYS:NZ	1.91	0.69
2:C:69:MET:O	2:C:73:LEU:HB2	1.93	0.69
1:A:113:THR:HG23	1:A:371:ASP:OD2	1.93	0.68
1:B:97:MET:HB3	1:B:122:MET:CE	2.22	0.68
1:A:1:MET:H3	1:A:352:LYS:HZ1	1.42	0.68
1:B:120:TYR:CE2	1:B:356:MET:HE2	2.28	0.68
1:A:296:GLU:HB2	5:A:420:HOH:O	1.94	0.68
1:A:244:ARG:HH11	1:A:244:ARG:HG2	1.59	0.68
1:B:120:TYR:OH	1:B:356:MET:HG3	1.94	0.68
2:C:194:MET:O	2:C:198:ILE:HG13	1.93	0.68
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.59	0.67
2:C:51:ILE:HG21	2:C:66:LEU:HD21	1.77	0.67
1:B:2:LYS:CE	1:B:34:ILE:HD11	2.23	0.67
1:A:332:SER:HB2	1:A:333:PRO:HD3	1.77	0.67
2:C:111:GLU:HB2	5:C:305:HOH:O	1.94	0.67
1:A:135:ASP:OD2	3:A:400:NAD:H4N	1.95	0.66
1:B:192:LYS:HE2	1:B:215:GLY:HA3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:MET:HE3	2:C:49:VAL:HG11	1.76	0.66
2:C:133:VAL:HG13	5:C:308:HOH:O	1.95	0.66
2:C:198:ILE:O	2:C:202:MET:HE3	1.96	0.66
1:A:244:ARG:HG2	1:A:244:ARG:NH1	2.10	0.65
1:B:374:ILE:HD12	1:B:374:ILE:H	1.61	0.65
1:A:221:VAL:HG23	1:A:247:GLN:HA	1.78	0.65
1:B:349:LYS:C	1:B:351:THR:N	2.28	0.65
1:A:278:GLU:HA	1:A:281:VAL:HG22	1.78	0.65
1:A:47:ASP:HB3	1:A:57:ILE:CD1	2.27	0.65
1:B:129:SER:HA	1:B:132:GLN:HE21	1.61	0.65
1:A:97:MET:HB3	1:A:122:MET:HE3	1.79	0.65
1:A:275:LEU:HD12	1:A:300:ASN:CB	2.23	0.65
1:B:3:ILE:HG13	1:B:70:VAL:HG12	1.79	0.65
1:A:176:LEU:HD23	1:A:199:MET:HB3	1.77	0.65
2:C:146:ILE:HG12	2:C:146:ILE:O	1.97	0.65
2:C:161:LEU:HD12	2:C:185:MET:HB2	1.78	0.65
1:A:80:ALA:HB2	1:A:85:ASP:HB2	1.78	0.64
2:C:129:GLY:O	4:C:300:NAP:H4B	1.97	0.64
1:B:224:GLU:O	1:B:225:ALA:HB2	1.96	0.64
1:A:307:GLY:H	1:A:321:THR:HG23	1.61	0.64
1:B:226:MET:CE	1:B:244:ARG:NH2	2.61	0.64
2:C:182:ASN:CG	2:C:183:ASN:N	2.55	0.64
1:B:226:MET:CE	1:B:244:ARG:HH22	2.11	0.64
2:C:85:HIS:HE1	2:C:87:VAL:HG22	1.63	0.64
1:A:158:ARG:HG2	1:B:329:ALA:CB	2.26	0.64
1:A:342:PHE:CE1	1:A:362:THR:HG22	2.32	0.63
1:A:178:PHE:CE2	1:A:276:ILE:HD11	2.32	0.63
2:C:159:THR:HA	2:C:183:ASN:HB3	1.81	0.63
2:C:140:THR:HG22	2:C:141:ASP:N	2.13	0.63
2:C:40:ALA:O	2:C:44:LYS:HB2	1.97	0.63
2:C:187:LEU:C	2:C:194:MET:HE3	2.23	0.63
1:A:343:LEU:C	1:A:343:LEU:HD23	2.23	0.62
2:C:141:ASP:C	2:C:143:SER:H	2.06	0.62
1:B:312:LYS:HG2	1:B:313:HIS:CD2	2.34	0.62
1:A:180:VAL:HG11	1:A:211:VAL:HG23	1.80	0.62
1:A:87:VAL:HG12	1:A:115:ARG:HG3	1.82	0.62
1:B:10:ARG:HH11	1:B:10:ARG:CG	2.09	0.62
1:B:224:GLU:CG	1:B:225:ALA:N	2.60	0.62
1:B:351:THR:O	1:B:351:THR:CG2	2.46	0.62
2:C:190:ASP:HB3	2:C:193:LYS:HD2	1.80	0.62
1:A:120:TYR:HB3	1:A:366:THR:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:187:LEU:O	2:C:194:MET:HE3	2.00	0.62
1:A:269:GLY:O	1:A:270:LYS:HG2	1.99	0.61
1:B:316:LYS:HG3	5:B:417:HOH:O	1.99	0.61
1:A:156:PHE:CZ	1:A:158:ARG:HB2	2.35	0.61
1:A:13:GLU:OE2	1:A:15:ARG:HB2	2.00	0.61
1:A:177:VAL:HG11	1:A:188:ILE:CG1	2.31	0.61
1:B:224:GLU:OE1	1:B:226:MET:SD	2.58	0.61
2:C:190:ASP:O	2:C:194:MET:HB2	2.01	0.60
1:A:307:GLY:N	1:A:321:THR:HG23	2.15	0.60
1:B:85:ASP:OD2	1:B:88:ALA:HB2	2.02	0.60
2:C:63:GLN:HG3	2:C:98:LEU:HB3	1.84	0.60
2:C:124:VAL:HG22	2:C:159:THR:HG23	1.84	0.60
1:A:184:GLY:O	1:A:188:ILE:HG13	2.01	0.60
1:B:125:MET:HE3	1:B:134:MET:HB3	1.83	0.60
1:B:222:ASP:HA	1:B:224:GLU:HG3	1.82	0.60
1:A:105:ASN:O	1:A:108:VAL:HG12	2.02	0.60
2:C:182:ASN:CG	2:C:183:ASN:H	2.09	0.60
1:B:6:PRO:HB3	1:B:65:LEU:HD11	1.83	0.60
1:B:18:ILE:HG13	1:B:19:SER:H	1.67	0.60
2:C:53:PRO:CB	2:C:95:MET:HE2	2.25	0.59
1:A:132:GLN:HG2	3:A:400:NAD:O7N	2.02	0.59
1:B:156:PHE:CE2	1:B:158:ARG:HB2	2.37	0.59
1:A:188:ILE:HG23	1:A:198:VAL:HG11	1.83	0.59
1:A:105:ASN:C	1:A:107:PRO:HD2	2.28	0.59
1:B:374:ILE:HD12	1:B:374:ILE:N	2.17	0.59
1:A:178:PHE:HE2	1:A:276:ILE:HD11	1.68	0.59
1:A:106:ARG:N	1:A:107:PRO:CD	2.66	0.59
1:A:177:VAL:HG11	1:A:188:ILE:HG12	1.83	0.59
1:A:244:ARG:HH11	1:A:244:ARG:CG	2.15	0.59
1:A:264:THR:HG22	1:A:293:LEU:HD12	1.85	0.59
1:A:4:ALA:C	1:A:5:ILE:HD12	2.28	0.58
1:B:199:MET:HE3	1:B:254:GLU:OE1	2.03	0.58
2:C:55:TYR:O	2:C:59:VAL:HG23	2.03	0.58
1:A:5:ILE:HD12	1:A:5:ILE:N	2.17	0.58
1:A:60:THR:HG23	1:A:63:GLN:H	1.68	0.58
1:A:110:GLU:O	1:A:114:LYS:HD3	2.03	0.58
2:C:169:SER:OG	2:C:173:GLY:HA2	2.04	0.58
1:B:221:VAL:CG1	1:B:247:GLN:HA	2.34	0.58
1:B:351:THR:O	1:B:352:LYS:CB	2.52	0.58
1:B:1:MET:H3	1:B:1:MET:HE3	1.67	0.58
1:B:161:PRO:HG2	1:B:163:MET:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:85:HIS:CG	2:C:133:VAL:HG22	2.38	0.58
1:B:224:GLU:OE1	1:B:225:ALA:N	2.37	0.57
1:A:1:MET:N	1:A:352:LYS:NZ	2.51	0.57
1:B:350:ASP:C	1:B:352:LYS:N	2.62	0.57
2:C:170:GLY:HA3	4:C:300:NAP:O1A	2.04	0.57
1:A:23:VAL:O	1:A:27:VAL:HG23	2.04	0.57
1:A:22:VAL:HG22	1:A:340:LEU:HD22	1.87	0.57
1:B:142:ASN:HD21	1:B:186:GLN:HE21	1.50	0.57
1:B:376:HIS:CE1	1:B:378:ALA:HB3	2.38	0.57
1:B:224:GLU:OE2	1:B:226:MET:SD	2.62	0.57
2:C:43:MET:HE1	2:C:69:MET:CE	2.35	0.57
1:A:87:VAL:CG1	1:A:112:LEU:HD23	2.33	0.57
1:A:72:TRP:HE1	1:A:97:MET:HE3	1.70	0.57
2:C:192:LYS:O	2:C:196:GLU:HB2	2.05	0.57
1:B:379:LEU:O	1:B:381:GLY:N	2.38	0.57
2:C:99:LEU:O	2:C:104:VAL:HG12	2.05	0.57
2:C:124:VAL:HG22	2:C:159:THR:CG2	2.35	0.56
2:C:144:SER:OG	2:C:146:ILE:HG22	2.05	0.56
1:B:122:MET:HE3	1:B:339:LEU:CD1	2.35	0.56
1:A:239:MET:SD	1:A:239:MET:CB	2.90	0.56
1:B:226:MET:CE	5:B:421:HOH:O	2.49	0.56
1:B:244:ARG:O	1:B:244:ARG:HG2	2.06	0.56
2:C:152:LEU:HB2	5:C:308:HOH:O	2.05	0.56
1:A:238:GLU:OE1	1:A:238:GLU:N	2.36	0.56
1:A:207:THR:HG22	1:A:218:PHE:CE1	2.40	0.56
2:C:69:MET:HG3	2:C:202:MET:HE1	1.86	0.56
1:A:70:VAL:HB	1:A:95:VAL:CG2	2.34	0.56
1:B:5:ILE:N	1:B:5:ILE:HD12	2.21	0.56
1:A:265:ALA:HB3	1:A:275:LEU:HD11	1.88	0.56
1:B:180:VAL:HG23	1:B:202:ASP:HB2	1.88	0.56
1:A:121:ALA:HB1	1:A:123:GLU:OE2	2.06	0.55
1:A:308:LYS:NZ	1:A:308:LYS:HB3	2.21	0.55
1:B:349:LYS:O	1:B:350:ASP:CB	2.52	0.55
1:A:276:ILE:HA	1:A:280:MET:HE3	1.86	0.55
1:B:160:PHE:N	1:B:161:PRO:HD2	2.21	0.55
1:A:44:SER:HA	5:A:407:HOH:O	2.07	0.55
1:B:243:PHE:C	1:B:245:LYS:H	2.13	0.55
2:C:203:ASN:OXT	2:C:203:ASN:O	2.22	0.55
1:A:85:ASP:OD2	1:A:88:ALA:HB2	2.06	0.55
1:A:129:SER:C	1:A:131:ALA:H	2.13	0.55
1:A:65:LEU:HD22	1:A:65:LEU:N	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:TYR:CE2	1:B:159:ALA:HA	2.41	0.55
1:A:269:GLY:C	1:A:270:LYS:HG2	2.31	0.55
1:A:279:GLU:O	1:A:282:THR:HG22	2.07	0.55
1:A:61:ALA:O	1:A:65:LEU:HD22	2.07	0.54
2:C:48:LYS:HD2	2:C:121:THR:O	2.05	0.54
1:B:51:THR:HA	1:B:55:ALA:O	2.06	0.54
1:B:322:ASN:HB3	5:B:389:HOH:O	2.06	0.54
1:B:282:THR:HG22	1:B:313:HIS:CE1	2.42	0.54
1:A:7:LYS:CG	1:A:39:ALA:HA	2.32	0.54
1:A:120:TYR:HE2	1:A:363:VAL:HG13	1.73	0.54
1:A:311:VAL:O	1:A:312:LYS:HG2	2.07	0.54
2:C:110:PHE:HB2	2:C:115:ILE:HD12	1.90	0.54
2:C:203:ASN:OXT	2:C:203:ASN:CB	2.56	0.53
1:B:178:PHE:CE1	1:B:276:ILE:HD11	2.44	0.53
1:B:224:GLU:CD	1:B:226:MET:SD	2.92	0.53
1:A:3:ILE:HG22	1:A:31:PHE:HB3	1.89	0.53
1:A:178:PHE:HB2	1:A:263:THR:HA	1.89	0.53
1:B:222:ASP:OD1	1:B:226:MET:HG2	2.09	0.53
1:A:47:ASP:HB3	1:A:57:ILE:HD13	1.90	0.53
1:B:275:LEU:HB2	1:B:300:ASN:HB3	1.89	0.53
1:B:350:ASP:HB2	1:B:353:THR:OG1	2.09	0.53
1:A:202:ASP:HB3	1:A:207:THR:HG21	1.89	0.53
1:B:349:LYS:O	1:B:349:LYS:HD2	2.09	0.53
1:A:313:HIS:N	1:A:313:HIS:CD2	2.77	0.52
1:B:108:VAL:HG13	1:B:109:VAL:N	2.24	0.52
1:A:346:HIS:HD2	1:A:357:LYS:H	1.56	0.52
1:B:128:ILE:HG13	1:B:128:ILE:O	2.09	0.52
1:B:208:LYS:HG2	1:B:212:GLU:OE2	2.09	0.52
2:C:85:HIS:CD2	2:C:112:LEU:HD12	2.44	0.52
1:A:95:VAL:HA	1:A:118:THR:O	2.09	0.52
1:A:114:LYS:HD2	1:A:114:LYS:N	2.23	0.52
1:A:367:CYS:SG	1:A:370:ARG:HB3	2.50	0.52
1:B:180:VAL:HG12	1:B:180:VAL:O	2.08	0.52
1:B:368:VAL:HG13	1:B:379:LEU:HD12	1.90	0.52
2:C:38:ASP:O	2:C:41:PHE:N	2.42	0.52
2:C:83:ALA:HB1	2:C:152:LEU:HD22	1.91	0.52
1:A:177:VAL:O	1:A:177:VAL:HG13	2.10	0.52
1:A:348:ASP:OD2	1:A:353:THR:HG23	2.09	0.52
1:A:281:VAL:HG23	1:A:282:THR:N	2.25	0.52
1:B:88:ALA:HA	1:B:115:ARG:NE	2.24	0.52
1:B:291:ILE:HD13	1:B:318:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:40:ALA:HB3	5:C:301:HOH:O	2.09	0.52
2:C:61:GLN:HG3	2:C:63:GLN:HE22	1.75	0.52
2:C:203:ASN:OXT	2:C:203:ASN:CA	2.53	0.52
2:C:160:VAL:HG11	2:C:162:PHE:HE1	1.75	0.51
2:C:176:ASN:O	2:C:179:PHE:HB2	2.10	0.51
1:A:326:ARG:HG2	1:A:326:ARG:NH1	2.24	0.51
1:B:19:SER:O	1:B:23:VAL:HG23	2.10	0.51
1:A:294:ALA:HB3	1:A:300:ASN:OD1	2.11	0.51
1:B:350:ASP:O	1:B:353:THR:HG23	2.11	0.51
2:C:44:LYS:HE2	2:C:202:MET:O	2.10	0.51
2:C:140:THR:O	2:C:142:PRO:HD3	2.11	0.51
2:C:142:PRO:HA	2:C:147:TYR:CD2	2.45	0.51
2:C:34:GLY:HA3	2:C:185:MET:CE	2.40	0.51
2:C:119:PHE:CD2	2:C:154:VAL:HA	2.45	0.51
1:A:10:ARG:HG3	5:A:417:HOH:O	2.10	0.51
1:A:97:MET:O	1:A:98:CYS:HB3	2.09	0.51
2:C:82:TYR:CE1	2:C:104:VAL:HG21	2.46	0.51
2:C:84:ILE:HD11	2:C:99:LEU:HD11	1.92	0.51
1:A:65:LEU:H	1:A:65:LEU:CD2	2.14	0.51
1:B:374:ILE:H	1:B:374:ILE:CD1	2.21	0.51
1:A:163:MET:HB2	1:A:170:VAL:HG13	1.92	0.51
1:A:5:ILE:HG12	1:A:18:ILE:HB	1.93	0.51
1:A:274:VAL:HG13	1:A:274:VAL:O	2.10	0.50
2:C:78:VAL:HG12	2:C:79:GLU:N	2.25	0.50
1:B:277:THR:OG1	1:B:280:MET:HG3	2.11	0.50
1:A:3:ILE:CG1	1:A:70:VAL:HG22	2.37	0.50
1:A:106:ARG:O	1:A:106:ARG:HD3	2.12	0.50
1:B:102:ALA:C	1:B:104:THR:H	2.19	0.50
1:B:263:THR:HG21	1:B:276:ILE:HD13	1.94	0.50
1:B:120:TYR:HD1	1:B:366:THR:HG23	1.76	0.50
2:C:158:GLY:O	2:C:183:ASN:OD1	2.30	0.50
1:A:18:ILE:HG13	1:A:19:SER:N	2.27	0.50
1:A:16:VAL:HG22	1:A:18:ILE:HG22	1.94	0.50
1:B:31:PHE:HE1	1:B:347:VAL:HG21	1.77	0.50
1:A:165:THR:CG2	2:C:92:PRO:HB3	2.42	0.49
1:B:51:THR:C	1:B:53:ALA:H	2.20	0.49
1:A:45:ILE:CG2	1:A:50:LEU:HD13	2.42	0.49
1:B:106:ARG:N	1:B:107:PRO:CD	2.75	0.49
1:B:349:LYS:C	1:B:350:ASP:CG	2.70	0.49
1:A:323:VAL:HB	1:A:324:PRO:HD3	1.93	0.49
1:B:246:LYS:HE2	1:B:249:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:48:LYS:HA	2:C:79:GLU:HB3	1.94	0.49
1:A:356:MET:O	1:A:358:LEU:N	2.45	0.49
1:B:160:PHE:CZ	1:B:260:ILE:HD12	2.46	0.49
1:B:320:HIS:HA	5:B:411:HOH:O	2.11	0.49
2:C:191:ALA:HB2	4:C:300:NAP:H2A	1.94	0.49
1:A:291:ILE:HD13	1:A:318:VAL:HB	1.94	0.49
1:B:192:LYS:HG3	5:B:420:HOH:O	2.13	0.49
2:C:112:LEU:HD23	2:C:112:LEU:O	2.12	0.49
2:C:119:PHE:CE2	2:C:154:VAL:HG12	2.48	0.49
1:B:3:ILE:HA	1:B:70:VAL:O	2.13	0.49
2:C:66:LEU:HD13	2:C:128:ILE:HG21	1.94	0.49
2:C:185:MET:HB3	2:C:187:LEU:CD1	2.43	0.49
1:A:256:VAL:O	1:A:285:LYS:HG3	2.13	0.48
1:B:30:GLY:CA	1:B:352:LYS:HE2	2.43	0.48
1:B:376:HIS:HE1	1:B:378:ALA:HB3	1.77	0.48
2:C:70:ALA:O	2:C:74:LYS:HG2	2.13	0.48
1:B:349:LYS:C	1:B:349:LYS:HD2	2.38	0.48
1:A:35:VAL:HG11	1:A:50:LEU:HD23	1.94	0.48
1:B:188:ILE:HG23	1:B:198:VAL:HG11	1.94	0.48
1:B:293:LEU:CD2	1:B:323:VAL:HG21	2.44	0.48
1:A:135:ASP:OD1	1:A:137:LEU:HB2	2.13	0.48
1:A:152:GLY:HA2	1:A:291:ILE:HD11	1.96	0.48
1:A:332:SER:O	1:A:333:PRO:C	2.56	0.48
2:C:49:VAL:HG22	2:C:124:VAL:HB	1.96	0.48
1:B:65:LEU:O	1:B:66:SER:C	2.57	0.48
1:A:23:VAL:HG11	1:A:55:ALA:HB2	1.95	0.48
1:A:3:ILE:HA	1:A:70:VAL:O	2.13	0.48
1:A:72:TRP:HE1	1:A:97:MET:CE	2.26	0.48
1:A:118:THR:HG23	1:A:370:ARG:HA	1.96	0.48
1:B:269:GLY:O	1:B:270:LYS:HD2	2.13	0.48
2:C:154:VAL:HG23	2:C:178:LEU:CD1	2.41	0.48
1:A:4:ALA:HA	1:A:34:ILE:O	2.14	0.48
1:A:357:LYS:O	1:A:359:GLU:N	2.44	0.47
1:A:120:TYR:OH	1:A:356:MET:HG3	2.14	0.47
2:C:160:VAL:HG11	2:C:162:PHE:CE1	2.48	0.47
1:B:1:MET:SD	1:B:354:LEU:HD22	2.54	0.47
1:A:207:THR:CG2	1:A:218:PHE:HE1	2.27	0.47
1:A:305:GLU:OE1	1:A:308:LYS:HD2	2.14	0.47
1:B:367:CYS:O	1:B:376:HIS:HB2	2.15	0.47
1:B:10:ARG:HG3	1:B:10:ARG:NH1	2.19	0.47
1:B:35:VAL:HG21	1:B:50:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:CB	1:A:207:THR:HG21	2.45	0.47
1:B:362:THR:HG22	1:B:363:VAL:HG23	1.97	0.47
1:A:75:GLN:HE21	1:A:75:GLN:HB2	1.51	0.47
1:B:342:PHE:CZ	1:B:366:THR:HG21	2.50	0.47
1:A:102:ALA:O	1:A:104:THR:N	2.48	0.47
1:A:122:MET:HE1	1:A:342:PHE:CD2	2.49	0.47
1:B:221:VAL:HG22	1:B:247:GLN:HG2	1.97	0.47
2:C:134:THR:HG21	2:C:154:VAL:HG11	1.97	0.47
1:A:142:ASN:O	1:A:186:GLN:HG2	2.14	0.46
1:A:349:LYS:HE3	1:A:349:LYS:HA	1.97	0.46
1:B:35:VAL:HG21	1:B:50:LEU:HD23	1.97	0.46
2:C:35:SER:O	2:C:38:ASP:HB2	2.16	0.46
2:C:66:LEU:CD1	2:C:128:ILE:HG21	2.45	0.46
2:C:141:ASP:O	2:C:143:SER:N	2.47	0.46
1:A:265:ALA:HA	3:A:400:NAD:O4B	2.15	0.46
1:B:1:MET:HE3	1:B:1:MET:N	2.31	0.46
1:B:6:PRO:HD2	1:B:72:TRP:O	2.16	0.46
1:B:222:ASP:OD1	1:B:225:ALA:HA	2.15	0.46
1:B:301:CYS:HA	1:B:302:PRO:HD2	1.78	0.46
1:A:59:SER:HB2	1:A:63:GLN:NE2	2.30	0.46
1:A:244:ARG:HD2	1:A:274:VAL:CG1	2.46	0.46
1:B:221:VAL:CG2	1:B:244:ARG:HH21	2.28	0.46
1:B:373:ALA:O	1:B:375:VAL:HG23	2.16	0.46
1:B:284:MET:CE	1:B:290:ILE:HD11	2.43	0.46
2:C:31:VAL:HG13	2:C:186:MET:HG3	1.96	0.46
1:A:247:GLN:C	1:A:249:GLU:N	2.73	0.46
1:A:327:VAL:O	1:A:327:VAL:HG12	2.16	0.46
2:C:52:VAL:HG12	2:C:52:VAL:O	2.15	0.46
1:A:267:ILE:O	1:A:268:PRO:C	2.58	0.46
1:B:178:PHE:CZ	1:B:276:ILE:HD11	2.51	0.46
2:C:85:HIS:CD2	2:C:133:VAL:HG22	2.50	0.46
2:C:169:SER:HB2	5:C:302:HOH:O	2.15	0.46
1:A:72:TRP:CD2	1:A:339:LEU:HD13	2.51	0.46
1:B:350:ASP:C	1:B:352:LYS:H	2.23	0.46
1:A:308:LYS:HB3	1:A:308:LYS:HZ3	1.80	0.46
1:B:224:GLU:CG	1:B:225:ALA:H	2.28	0.46
1:B:315:VAL:O	1:B:317:ILE:HD12	2.15	0.46
2:C:142:PRO:HB3	2:C:147:TYR:CZ	2.51	0.46
1:A:256:VAL:HG12	1:A:283:LYS:O	2.15	0.45
2:C:53:PRO:HB3	2:C:57:MET:HE3	1.98	0.45
2:C:57:MET:HE2	2:C:66:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:162:PHE:CD2	2:C:179:PHE:HE1	2.34	0.45
1:A:60:THR:HG23	1:A:63:GLN:HB2	1.99	0.45
1:A:72:TRP:CG	1:A:339:LEU:HD13	2.52	0.45
1:A:140:GLN:OE1	1:A:331:ALA:HB1	2.16	0.45
1:B:7:LYS:HG3	1:B:39:ALA:HA	1.98	0.45
1:B:275:LEU:C	1:B:276:ILE:HD12	2.41	0.45
1:B:128:ILE:O	1:B:130:ARG:N	2.50	0.45
1:B:149:VAL:HG21	1:B:190:THR:HB	1.98	0.45
1:B:265:ALA:HB3	1:B:300:ASN:ND2	2.32	0.45
1:B:320:HIS:HB3	5:B:410:HOH:O	2.17	0.45
2:C:63:GLN:CG	2:C:98:LEU:HB3	2.46	0.45
1:A:106:ARG:NH1	1:A:110:GLU:HB3	2.32	0.45
1:A:239:MET:HB3	1:A:243:PHE:CG	2.52	0.45
1:B:122:MET:HE3	1:B:339:LEU:HD12	1.99	0.45
1:B:156:PHE:CZ	1:B:259:ASP:HB3	2.52	0.45
1:B:226:MET:HE1	1:B:244:ARG:CZ	2.47	0.45
1:B:323:VAL:O	1:B:326:ARG:HB2	2.16	0.45
2:C:123:ASP:O	2:C:159:THR:HG22	2.17	0.45
1:B:252:LEU:C	1:B:252:LEU:HD13	2.42	0.45
1:B:295:VAL:HG11	1:B:319:GLY:O	2.16	0.45
1:A:136:ILE:O	1:A:140:GLN:HG2	2.17	0.44
1:B:70:VAL:HG22	1:B:95:VAL:HB	1.99	0.44
2:C:164:LYS:O	2:C:188:PHE:HA	2.18	0.44
1:A:344:THR:HB	1:A:345:PRO:HD3	2.00	0.44
1:B:51:THR:C	1:B:53:ALA:N	2.72	0.44
1:B:143:LEU:HD11	1:B:334:LEU:HD12	1.98	0.44
1:B:246:LYS:HD2	1:B:246:LYS:HA	1.79	0.44
2:C:140:THR:HG22	2:C:141:ASP:H	1.79	0.44
2:C:34:GLY:HA3	2:C:185:MET:HE1	1.98	0.44
1:A:97:MET:HE1	1:A:343:LEU:CD1	2.39	0.44
1:A:178:PHE:CD2	1:A:263:THR:HG22	2.52	0.44
1:A:337:LYS:HE3	1:A:337:LYS:HB2	1.83	0.44
1:B:10:ARG:CG	1:B:10:ARG:NH1	2.72	0.44
1:B:105:ASN:O	1:B:108:VAL:HG12	2.18	0.44
1:B:208:LYS:HG3	1:B:218:PHE:CB	2.47	0.44
1:B:221:VAL:HG12	1:B:250:ALA:HB2	2.00	0.44
1:B:224:GLU:HG3	1:B:225:ALA:N	2.33	0.44
1:B:282:THR:HG22	1:B:313:HIS:ND1	2.33	0.44
1:B:295:VAL:CG1	1:B:296:GLU:N	2.80	0.44
1:B:359:GLU:N	1:B:359:GLU:CD	2.76	0.44
1:A:122:MET:HB2	1:A:136:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PHE:CE2	1:A:158:ARG:HB2	2.53	0.44
1:B:224:GLU:OE1	1:B:225:ALA:C	2.61	0.44
1:B:246:LYS:HE2	1:B:249:GLU:CG	2.47	0.44
1:A:276:ILE:O	1:A:302:PRO:HD2	2.18	0.44
1:B:243:PHE:C	1:B:245:LYS:N	2.76	0.44
1:A:180:VAL:HG11	1:A:211:VAL:CG2	2.46	0.43
1:A:232:ALA:C	1:A:234:GLY:H	2.25	0.43
1:B:122:MET:HB3	1:B:136:ILE:HD13	1.99	0.43
2:C:72:VAL:HA	2:C:75:LYS:HB2	1.99	0.43
1:A:203:VAL:HG11	1:A:239:MET:HG3	1.99	0.43
1:A:204:ARG:O	1:A:207:THR:HB	2.18	0.43
1:B:4:ALA:HA	1:B:34:ILE:O	2.18	0.43
1:B:120:TYR:CZ	1:B:356:MET:HE2	2.52	0.43
1:A:207:THR:HG22	1:A:208:LYS:N	2.33	0.43
1:A:305:GLU:O	1:A:308:LYS:HG2	2.18	0.43
1:B:317:ILE:HD12	1:B:317:ILE:N	2.34	0.43
1:A:61:ALA:O	1:A:65:LEU:CD2	2.66	0.43
1:B:256:VAL:O	1:B:256:VAL:HG12	2.18	0.43
2:C:187:LEU:HB3	2:C:194:MET:CE	2.49	0.43
2:C:203:ASN:OXT	2:C:203:ASN:HB2	2.19	0.43
1:A:364:SER:OG	1:A:365:GLY:N	2.51	0.43
1:B:220:THR:HB	5:B:421:HOH:O	2.18	0.43
2:C:78:VAL:CG1	2:C:79:GLU:N	2.81	0.43
1:A:35:VAL:HG11	1:A:50:LEU:CD2	2.49	0.43
1:A:129:SER:C	1:A:131:ALA:N	2.77	0.43
1:A:343:LEU:C	1:A:343:LEU:CD2	2.91	0.43
2:C:97:VAL:HG13	2:C:98:LEU:N	2.33	0.43
2:C:140:THR:CG2	2:C:141:ASP:H	2.32	0.43
1:B:50:LEU:HD12	1:B:50:LEU:HA	1.83	0.43
1:B:184:GLY:O	1:B:188:ILE:HG13	2.18	0.43
2:C:146:ILE:CG1	2:C:149:MET:HE2	2.49	0.43
1:A:280:MET:O	1:A:281:VAL:C	2.62	0.43
2:C:119:PHE:CG	2:C:153:ASP:O	2.71	0.43
1:A:221:VAL:O	1:A:222:ASP:HB2	2.18	0.43
1:B:30:GLY:O	1:B:352:LYS:HD3	2.19	0.43
1:B:243:PHE:CE1	1:B:245:LYS:HE3	2.53	0.43
2:C:68:GLU:C	2:C:70:ALA:N	2.75	0.43
1:A:18:ILE:HG13	1:A:19:SER:H	1.84	0.43
1:A:74:VAL:HA	1:A:335:PHE:CE2	2.54	0.43
1:A:96:LEU:O	1:A:119:ALA:HA	2.19	0.43
1:A:312:LYS:HB3	1:A:313:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ALA:C	1:B:5:ILE:HD12	2.44	0.43
1:A:348:ASP:O	1:A:350:ASP:N	2.52	0.42
1:B:7:LYS:HD3	1:B:9:ARG:NH1	2.34	0.42
1:B:136:ILE:O	1:B:140:GLN:HG2	2.19	0.42
2:C:91:MET:HE2	2:C:94:HIS:HA	2.01	0.42
2:C:161:LEU:HD12	2:C:161:LEU:HA	1.78	0.42
1:A:10:ARG:NH2	1:A:76:ARG:HH22	2.16	0.42
1:A:221:VAL:CG2	1:A:222:ASP:N	2.67	0.42
1:A:235:TYR:HB2	1:A:236:ALA:H	1.70	0.42
1:B:295:VAL:HG13	1:B:296:GLU:N	2.33	0.42
1:B:92:GLU:OE2	1:B:116:LYS:HD2	2.20	0.42
1:B:226:MET:HE1	1:B:244:ARG:NH1	2.35	0.42
1:A:351:THR:O	1:A:353:THR:HG22	2.19	0.42
1:B:18:ILE:HG13	1:B:19:SER:N	2.32	0.42
1:B:26:LEU:O	1:B:27:VAL:C	2.63	0.42
2:C:187:LEU:HB3	2:C:194:MET:HE3	2.02	0.42
1:A:329:ALA:HB3	1:B:158:ARG:CG	2.46	0.42
1:B:102:ALA:C	1:B:104:THR:N	2.77	0.42
1:B:108:VAL:CG1	1:B:109:VAL:N	2.82	0.42
1:B:133:SER:HB2	1:B:341:ASN:ND2	2.34	0.42
1:A:10:ARG:NH2	1:A:76:ARG:NH2	2.67	0.42
1:B:135:ASP:OD1	1:B:137:LEU:HB2	2.19	0.42
1:B:125:MET:HA	1:B:126:PRO:HD3	1.90	0.42
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.93	0.42
2:C:178:LEU:O	2:C:184:THR:HG21	2.19	0.42
2:C:187:LEU:CD1	2:C:187:LEU:N	2.83	0.42
2:C:40:ALA:HB1	2:C:201:ALA:O	2.20	0.42
2:C:119:PHE:CB	2:C:153:ASP:O	2.68	0.42
2:C:136:PRO:C	2:C:138:ALA:H	2.28	0.42
1:A:279:GLU:OE2	1:A:283:LYS:HE3	2.20	0.41
1:A:295:VAL:HG23	1:A:304:SER:OG	2.19	0.41
1:A:317:ILE:N	1:A:317:ILE:HD12	2.35	0.41
1:B:59:SER:HB2	1:B:63:GLN:OE1	2.19	0.41
1:B:359:GLU:N	1:B:359:GLU:OE1	2.47	0.41
2:C:187:LEU:N	2:C:187:LEU:HD12	2.35	0.41
1:A:276:ILE:CA	1:A:280:MET:HE3	2.50	0.41
1:B:97:MET:CB	1:B:122:MET:HE1	2.32	0.41
1:A:103:LEU:CD1	1:A:103:LEU:H	2.33	0.41
1:B:275:LEU:HD23	1:B:275:LEU:HA	1.87	0.41
2:C:179:PHE:O	2:C:186:MET:HE3	2.20	0.41
1:A:192:LYS:HG2	1:A:198:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:PHE:N	1:B:161:PRO:CD	2.83	0.41
1:B:202:ASP:HB3	1:B:207:THR:HG21	2.02	0.41
2:C:71:ASP:HA	2:C:74:LYS:HG2	2.03	0.41
1:A:203:VAL:CB	1:A:239:MET:HE2	2.47	0.41
1:A:265:ALA:CB	1:A:275:LEU:HD11	2.50	0.41
1:B:81:GLU:O	1:B:81:GLU:HG3	2.20	0.41
1:B:85:ASP:CG	1:B:88:ALA:HB2	2.45	0.41
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.91	0.41
1:B:278:GLU:HG3	1:B:303:LEU:HD11	2.01	0.41
1:B:74:VAL:CG2	1:B:75:GLN:N	2.83	0.41
1:B:110:GLU:O	1:B:111:ALA:C	2.64	0.41
1:B:192:LYS:CE	1:B:215:GLY:HA3	2.47	0.41
1:B:303:LEU:O	1:B:310:VAL:HG11	2.21	0.41
2:C:43:MET:HE2	2:C:73:LEU:HD21	2.02	0.41
1:A:1:MET:N	1:A:352:LYS:HZ3	2.19	0.41
1:A:16:VAL:O	1:A:16:VAL:HG13	2.20	0.41
1:B:109:VAL:HG13	1:B:368:VAL:CG1	2.51	0.41
1:A:90:ILE:O	1:A:91:LYS:C	2.64	0.41
1:A:103:LEU:H	1:A:103:LEU:HD13	1.86	0.41
1:A:176:LEU:HD13	1:A:178:PHE:CZ	2.55	0.41
1:A:177:VAL:HG11	1:A:188:ILE:HD11	2.02	0.41
1:A:265:ALA:HB3	1:A:300:ASN:ND2	2.35	0.41
1:B:51:THR:O	1:B:53:ALA:N	2.54	0.41
1:B:349:LYS:C	1:B:349:LYS:CD	2.94	0.41
1:B:379:LEU:O	1:B:380:THR:C	2.64	0.41
2:C:61:GLN:HA	2:C:63:GLN:OE1	2.20	0.41
2:C:120:GLN:HG2	2:C:156:LYS:HD3	2.02	0.41
2:C:160:VAL:HB	2:C:184:THR:HA	2.03	0.41
1:A:73:LYS:NZ	5:A:422:HOH:O	2.54	0.41
1:A:86:GLU:C	1:A:88:ALA:N	2.78	0.41
1:B:18:ILE:HD12	1:B:18:ILE:HA	1.86	0.41
1:B:342:PHE:CE1	1:B:362:THR:HG23	2.56	0.41
2:C:141:ASP:C	2:C:143:SER:N	2.76	0.41
1:A:175:VAL:HG22	1:A:260:ILE:HB	2.03	0.40
1:A:232:ALA:HA	1:A:235:TYR:O	2.21	0.40
1:B:9:ARG:HD3	1:B:9:ARG:HA	1.83	0.40
1:B:104:THR:HG23	1:B:105:ASN:ND2	2.35	0.40
2:C:152:LEU:CB	5:C:308:HOH:O	2.68	0.40
1:A:203:VAL:HG12	1:A:243:PHE:CZ	2.56	0.40
2:C:53:PRO:C	2:C:95:MET:HE2	2.46	0.40
1:A:241:GLU:OE2	1:A:245:LYS:NZ	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ALA:C	1:B:207:THR:H	2.30	0.40
1:A:352:LYS:HE2	1:A:352:LYS:HB3	1.90	0.40
2:C:157:ALA:O	2:C:158:GLY:C	2.65	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	358/384 (93%)	295 (82%)	50 (14%)	13 (4%)	2	3
1	B	362/384 (94%)	317 (88%)	29 (8%)	16 (4%)	2	2
2	C	172/203 (85%)	138 (80%)	25 (14%)	9 (5%)	1	1
All	All	892/971 (92%)	750 (84%)	104 (12%)	38 (4%)	2	2

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ALA
1	A	103	LEU
1	A	349	LYS
1	A	357	LYS
1	B	66	SER
1	B	129	SER
1	B	224	GLU
1	B	225	ALA
1	B	351	THR
1	B	352	LYS
1	B	380	THR
2	C	182	ASN
1	A	221	VAL
1	B	243	PHE

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Mol	Chain	Res	Type
1	B	378	ALA
2	C	78	VAL
2	C	131	ASN
1	A	238	GLU
1	A	350	ASP
1	B	245	LYS
2	C	31	VAL
2	C	38	ASP
2	C	141	ASP
1	A	268	PRO
1	A	320	HIS
1	A	351	THR
1	A	358	LEU
1	B	103	LEU
1	B	306	PRO
2	C	112	LEU
2	C	115	ILE
1	B	350	ASP
1	B	377	PRO
2	C	142	PRO
1	A	90	ILE
1	A	248	ALA
1	B	52	ALA
1	B	302	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/296 (95%)	253 (90%)	29 (10%)	7	14
1	B	286/296 (97%)	252 (88%)	34 (12%)	5	11
2	C	138/154 (90%)	127 (92%)	11 (8%)	11	24
All	All	706/746 (95%)	632 (90%)	74 (10%)	6	14

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	24	LYS
1	A	31	PHE
1	A	37	GLN
1	A	50	LEU
1	A	60	THR
1	A	65	LEU
1	A	70	VAL
1	A	75	GLN
1	A	81	GLU
1	A	95	VAL
1	A	96	LEU
1	A	132	GLN
1	A	135	ASP
1	A	164	MET
1	A	170	VAL
1	A	176	LEU
1	A	207	THR
1	A	235	TYR
1	A	244	ARG
1	A	246	LYS
1	A	268	PRO
1	A	282	THR
1	A	301	CYS
1	A	308	LYS
1	A	313	HIS
1	A	324	PRO
1	A	349	LYS
1	A	353	THR
1	B	1	MET
1	B	10	ARG
1	B	29	LEU
1	B	32	GLU
1	B	35	VAL
1	B	73	LYS
1	B	74	VAL
1	B	89	LEU
1	B	106	ARG
1	B	115	ARG
1	B	127	ARG
1	B	137	LEU
1	B	147	ARG
1	B	176	LEU

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Mol	Chain	Res	Type
1	B	199	MET
1	B	210	GLN
1	B	222	ASP
1	B	223	ASP
1	B	224	GLU
1	B	242	GLU
1	B	243	PHE
1	B	247	GLN
1	B	270	LYS
1	B	276	ILE
1	B	281	VAL
1	B	289	VAL
1	B	327	VAL
1	B	337	LYS
1	B	339	LEU
1	B	349	LYS
1	B	350	ASP
1	B	351	THR
1	B	362	THR
1	B	369	THR
2	C	61	GLN
2	C	63	GLN
2	C	86	PRO
2	C	91	MET
2	C	104	VAL
2	C	106	TYR
2	C	133	VAL
2	C	161	LEU
2	C	178	LEU
2	C	194	MET
2	C	196	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	63	GLN
1	A	75	GLN
1	A	142	ASN
1	A	186	GLN
1	A	210	GLN
1	A	247	GLN

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Mol	Chain	Res	Type
1	A	313	HIS
1	A	346	HIS
1	B	67	GLN
1	B	132	GLN
1	B	142	ASN
1	B	186	GLN
1	B	341	ASN
1	B	376	HIS
2	C	45	ASN
2	C	120	GLN
2	C	183	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAP	C	300	-	50,52,52	2.06	11 (22%)	71,80,80	2.49	24 (33%)
3	NAD	A	400	-	46,48,48	3.14	14 (30%)	64,73,73	1.73	14 (21%)

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
4	NAP	C	300	-	-	10/35/67/67	0/5/5/5
3	NAD	A	400	-	-	13/30/62/62	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	NAD	O2D-C2D	-11.99	1.13	1.43
3	A	400	NAD	C5D-C4D	-7.85	1.28	1.51
4	C	300	NAP	C2N-N1N	7.63	1.43	1.35
4	C	300	NAP	PA-O3	6.61	1.66	1.59
3	A	400	NAD	C6N-N1N	6.38	1.49	1.35
3	A	400	NAD	C3N-C7N	6.01	1.59	1.50
3	A	400	NAD	C2N-N1N	5.77	1.41	1.35
3	A	400	NAD	C4N-C3N	5.49	1.47	1.39
3	A	400	NAD	PN-O3	-4.71	1.54	1.59
4	C	300	NAP	P2B-O2B	3.87	1.66	1.59
3	A	400	NAD	C2A-N1A	3.74	1.40	1.33
4	C	300	NAP	O4D-C1D	3.71	1.45	1.40
3	A	400	NAD	O4D-C1D	3.49	1.45	1.40
4	C	300	NAP	C6N-N1N	3.42	1.43	1.35
3	A	400	NAD	C4A-N3A	3.33	1.40	1.34
4	C	300	NAP	C5N-C4N	3.00	1.44	1.38
4	C	300	NAP	C4N-C3N	2.75	1.43	1.39
3	A	400	NAD	PN-O5D	-2.70	1.48	1.59
4	C	300	NAP	C5A-N7A	-2.69	1.34	1.39
4	C	300	NAP	C3N-C7N	2.50	1.54	1.50
3	A	400	NAD	C6A-N1A	2.47	1.42	1.35
4	C	300	NAP	C8A-N7A	2.45	1.36	1.31
3	A	400	NAD	C8A-N7A	2.27	1.36	1.31
3	A	400	NAD	C5N-C4N	2.14	1.42	1.38
4	C	300	NAP	C4A-N3A	2.07	1.38	1.34

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	300	NAP	O3-PA-O1A	-7.73	87.45	110.70
4	C	300	NAP	O2A-PA-O3	-7.39	87.31	107.27
4	C	300	NAP	N3A-C2A-N1A	-6.73	118.39	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	300	NAP	C5A-C4A-N3A	-5.04	119.77	126.72
3	A	400	NAD	O5D-C5D-C4D	4.89	125.64	108.99
4	C	300	NAP	N3A-C4A-N9A	4.53	134.88	127.17
3	A	400	NAD	C5N-C6N-N1N	-4.52	114.21	120.38
4	C	300	NAP	C2B-C1B-N9A	4.52	121.19	113.75
4	C	300	NAP	C2A-N3A-C4A	4.51	122.85	111.83
3	A	400	NAD	C6N-C5N-C4N	4.32	125.67	119.45
4	C	300	NAP	N9A-C8A-N7A	-4.22	107.95	113.94
3	A	400	NAD	O4B-C1B-C2B	-4.18	97.66	106.62
4	C	300	NAP	C3B-C2B-C1B	-3.98	95.18	102.81
4	C	300	NAP	O2A-PA-O1A	3.89	130.53	112.44
3	A	400	NAD	C4N-C3N-C7N	-3.71	110.95	121.06
4	C	300	NAP	C4A-N9A-C8A	3.44	109.36	105.74
4	C	300	NAP	C5N-C4N-C3N	3.41	123.72	120.36
4	C	300	NAP	C4A-N9A-C1B	-3.34	118.82	126.63
3	A	400	NAD	C5N-C4N-C3N	-3.33	117.09	120.36
3	A	400	NAD	O2A-PA-O3	3.07	115.58	107.27
3	A	400	NAD	C2N-C3N-C7N	3.03	128.21	119.46
3	A	400	NAD	C4B-O4B-C1B	-2.77	103.36	109.47
4	C	300	NAP	O4B-C1B-N9A	2.73	113.33	108.09
4	C	300	NAP	C2B-C3B-C4B	2.57	107.52	101.99
4	C	300	NAP	O4B-C4B-C3B	-2.55	100.10	105.15
3	A	400	NAD	C5D-C4D-C3D	-2.43	106.48	115.21
4	C	300	NAP	O2B-C2B-C1B	2.34	118.28	110.05
4	C	300	NAP	O3B-C3B-C4B	-2.32	104.41	111.08
3	A	400	NAD	O2B-C2B-C1B	2.31	118.05	110.10
4	C	300	NAP	C2D-C3D-C4D	2.29	107.04	102.61
4	C	300	NAP	C4D-O4D-C1D	2.23	111.96	109.92
3	A	400	NAD	C2N-C3N-C4N	2.22	120.84	118.26
4	C	300	NAP	C5B-C4B-C3B	-2.17	107.40	115.21
4	C	300	NAP	C6N-C5N-C4N	-2.14	116.37	119.45
4	C	300	NAP	O3D-C3D-C4D	-2.13	104.97	111.08
4	C	300	NAP	C1B-N9A-C8A	2.13	131.81	127.09
3	A	400	NAD	N3A-C2A-N1A	-2.06	125.46	128.58
3	A	400	NAD	C2B-C1B-N9A	2.04	118.37	113.30

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	NAD	C5B-O5B-PA-O1A
3	A	400	NAD	C5B-O5B-PA-O2A

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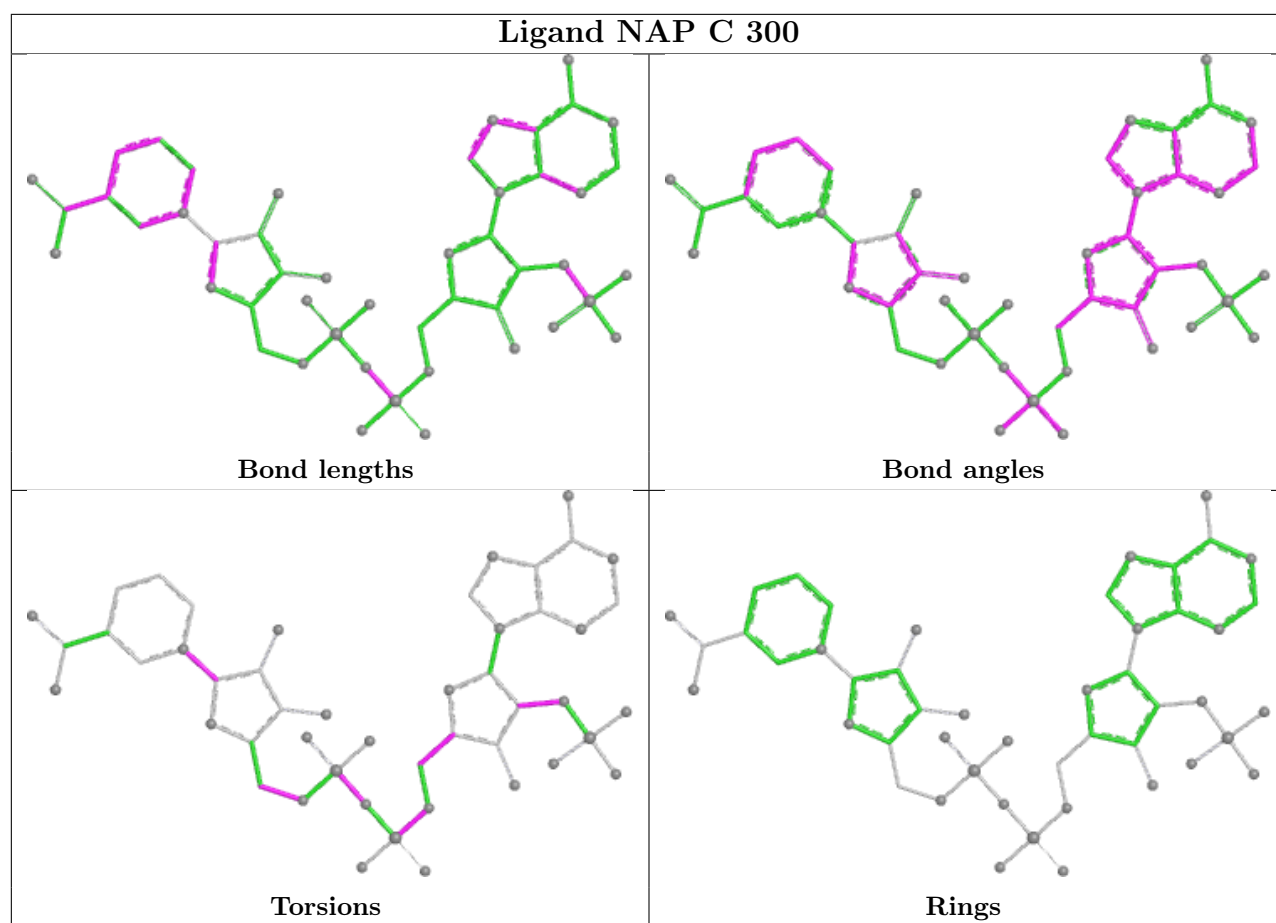
Mol	Chain	Res	Type	Atoms
3	A	400	NAD	C5B-O5B-PA-O3
4	C	300	NAP	C5B-O5B-PA-O1A
4	C	300	NAP	C5B-O5B-PA-O3
4	C	300	NAP	O4D-C1D-N1N-C2N
4	C	300	NAP	O4D-C1D-N1N-C6N
3	A	400	NAD	O4D-C4D-C5D-O5D
4	C	300	NAP	C1B-C2B-O2B-P2B
4	C	300	NAP	C3B-C4B-C5B-O5B
3	A	400	NAD	C3D-C4D-C5D-O5D
3	A	400	NAD	C2N-C3N-C7N-O7N
3	A	400	NAD	C2N-C3N-C7N-N7N
3	A	400	NAD	C3B-C4B-C5B-O5B
4	C	300	NAP	O4B-C4B-C5B-O5B
3	A	400	NAD	C4N-C3N-C7N-O7N
3	A	400	NAD	C4N-C3N-C7N-N7N
3	A	400	NAD	PN-O3-PA-O1A
4	C	300	NAP	PA-O3-PN-O2N
3	A	400	NAD	O4B-C4B-C5B-O5B
4	C	300	NAP	C4D-C5D-O5D-PN
4	C	300	NAP	PA-O3-PN-O1N
3	A	400	NAD	PN-O3-PA-O2A

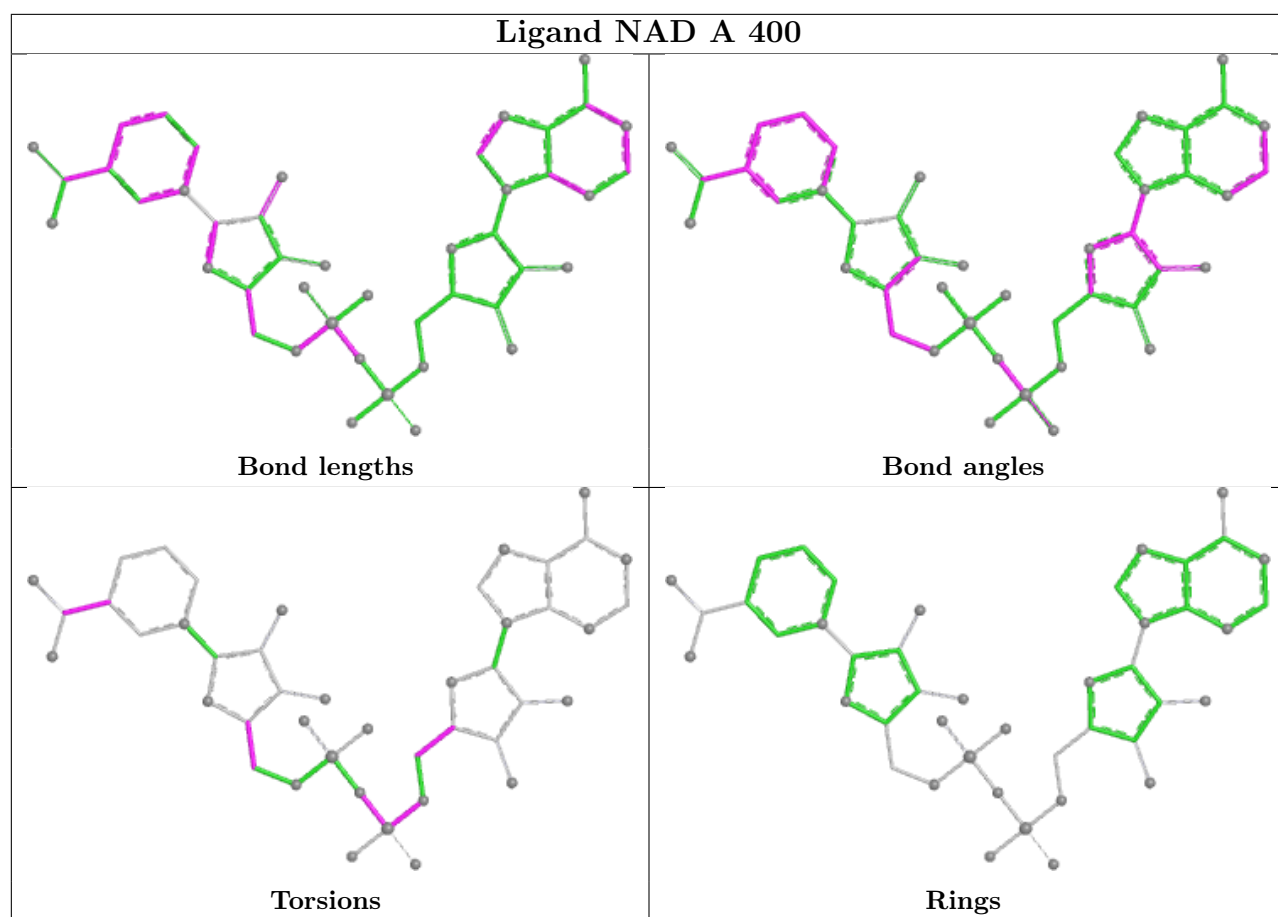
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	300	NAP	3	0
3	A	400	NAD	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.