



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:41 PM UTC

PDB ID : 1BI9 / pdb_00001bi9
Title : RETINAL DEHYDROGENASE TYPE TWO WITH NAD BOUND
Authors : Newcomer, M.E.; Lamb, A.L.
Deposited on : 1998-06-23
Resolution : 2.70 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

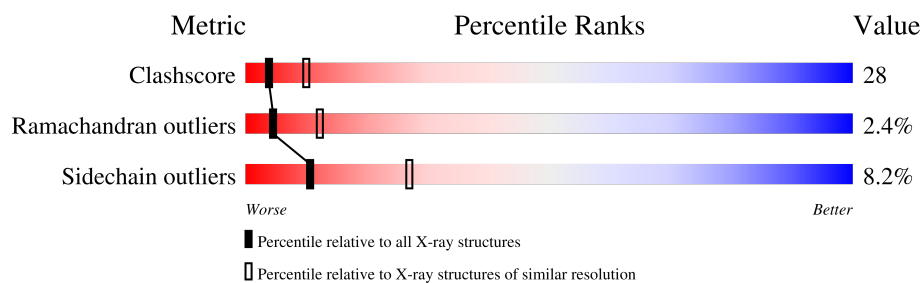
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	499	
1	B	499	
1	C	499	
1	D	499	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Cl	0	0
			2	2		

- Molecule 4 is water.

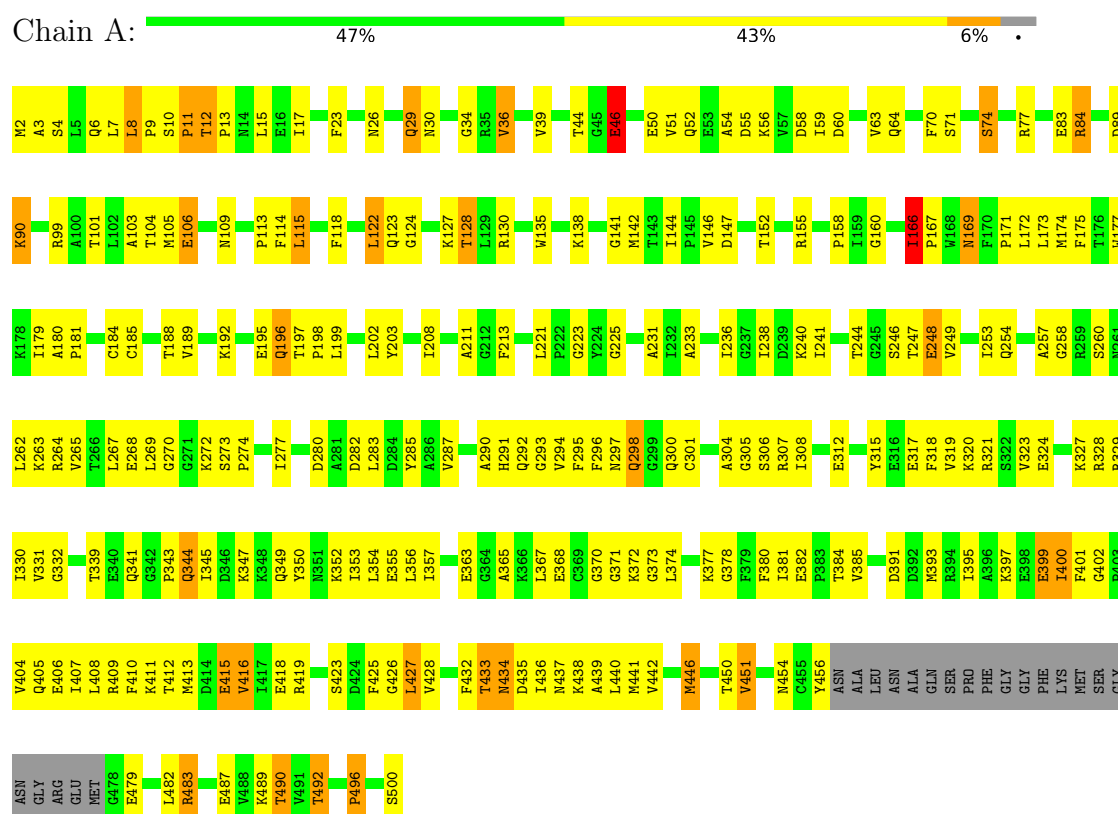
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	53	Total	O	0	0
			53	53		
4	C	68	Total	O	0	0
			68	68		
4	D	66	Total	O	0	0
			66	66		

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. 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.

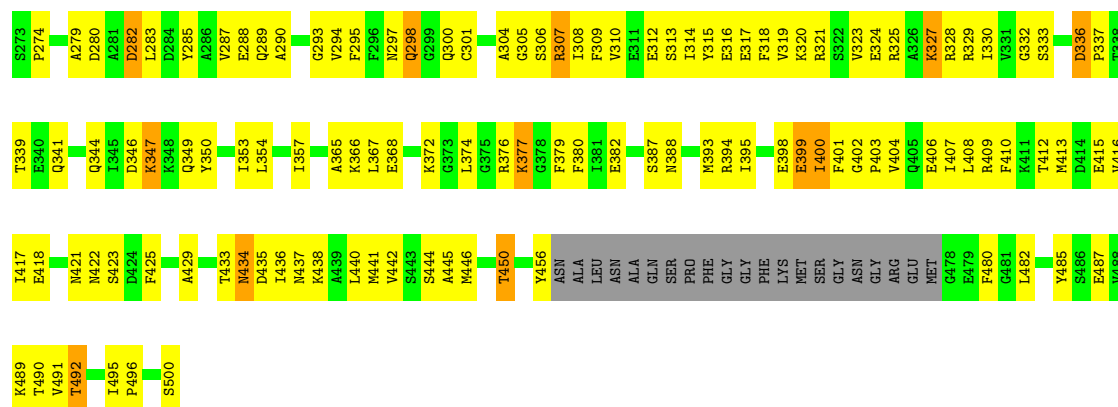
Note EDS was not executed.

• Molecule 1: RETINAL DEHYDROGENASE TYPE II



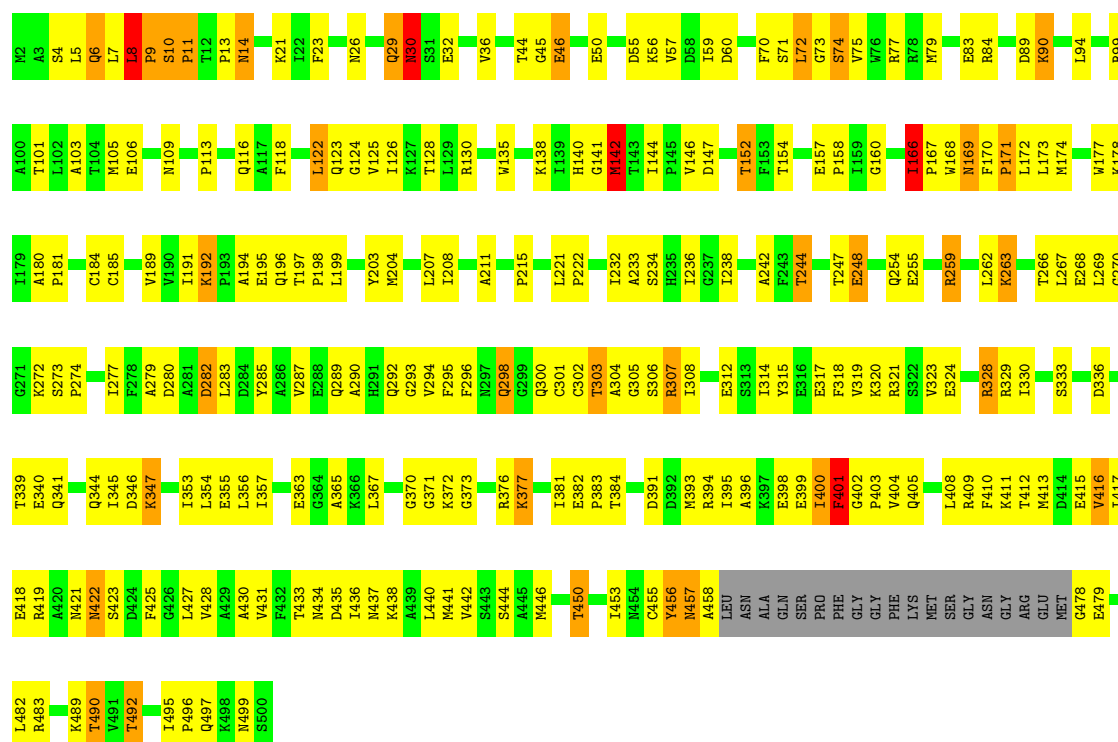
• Molecule 1: RETINAL DEHYDROGENASE TYPE II





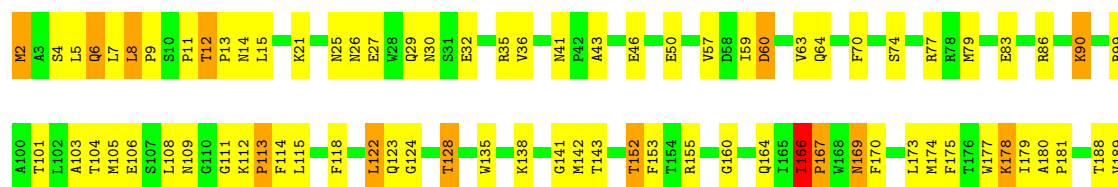
• Molecule 1: RETINAL DEHYDROGENASE TYPE II

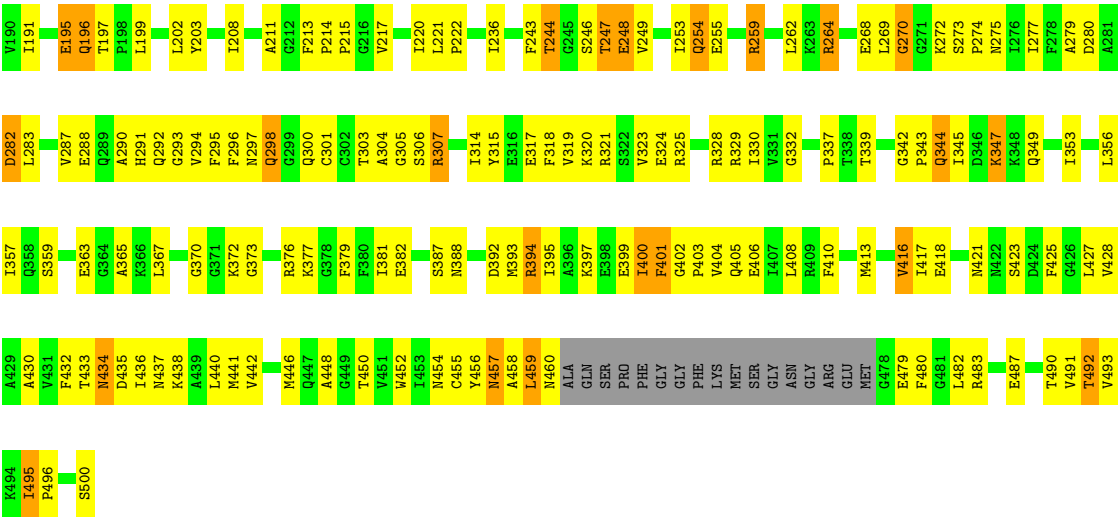
Chain C: 47% 41% 7%



• Molecule 1: RETINAL DEHYDROGENASE TYPE II

Chain D: 49% 40% 7%





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 2	Depositor
Cell constants a, b, c, α , β , γ	149.80Å 167.30Å 107.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	95.1 (30.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.234 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15156	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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, CL

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	0.47	0/3772	0.96	17/5104 (0.3%)
1	B	0.47	0/3764	0.95	15/5094 (0.3%)
1	C	0.52	0/3785	0.99	16/5122 (0.3%)
1	D	0.49	0/3801	0.99	18/5144 (0.3%)
All	All	0.49	0/15122	0.97	66/20464 (0.3%)

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	LYS	N-CA-C	-11.05	99.32	111.36
1	C	123	GLN	N-CA-C	-8.48	102.12	111.36
1	D	345	ILE	N-CA-C	8.02	118.80	110.62
1	B	141	GLY	N-CA-C	-7.92	101.72	112.57
1	D	199	LEU	N-CA-C	7.81	119.49	110.97
1	C	141	GLY	N-CA-C	-7.32	102.54	112.57
1	C	45	GLY	N-CA-C	-7.14	106.58	115.08
1	D	7	LEU	N-CA-C	-7.03	104.17	112.89
1	D	141	GLY	N-CA-C	-6.87	103.33	112.81
1	A	347	LYS	N-CA-C	-6.86	103.26	111.69
1	A	166	ILE	N-CA-C	6.83	115.42	107.84
1	C	142	MET	N-CA-C	6.67	119.08	109.14
1	A	189	VAL	N-CA-C	6.53	119.50	108.86
1	C	144	ILE	N-CA-C	6.53	115.18	107.73
1	D	123	GLN	N-CA-C	-6.28	104.52	111.36
1	C	345	ILE	N-CA-C	6.25	117.03	110.72
1	C	191	ILE	N-CA-C	6.17	117.47	108.53
1	B	140	HIS	N-CA-C	6.09	119.97	110.17
1	A	451	VAL	N-CA-C	6.07	116.67	108.17
1	B	434	ASN	N-CA-C	-6.06	103.99	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	ASN	N-CA-C	6.03	117.52	111.07
1	D	347	LYS	N-CA-C	-5.96	104.36	111.69
1	D	191	ILE	N-CA-C	5.96	116.51	108.17
1	D	434	ASN	N-CA-C	-5.95	104.69	113.61
1	C	166	ILE	N-CA-C	5.95	115.58	108.45
1	B	133	ALA	N-CA-C	-5.94	104.14	111.33
1	A	434	ASN	N-CA-C	-5.91	104.93	114.09
1	B	346	ASP	N-CA-C	5.90	118.14	109.24
1	A	141	GLY	N-CA-C	-5.86	104.22	112.60
1	C	189	VAL	N-CA-C	5.82	117.81	108.85
1	A	46	GLU	N-CA-C	5.81	118.05	110.43
1	B	189	VAL	N-CA-C	5.75	117.70	108.85
1	D	189	VAL	N-CA-C	5.73	117.00	108.46
1	B	347	LYS	N-CA-C	-5.73	105.11	111.36
1	B	166	ILE	N-CA-C	5.71	114.18	107.84
1	A	144	ILE	N-CA-C	5.65	114.05	107.89
1	B	188	THR	N-CA-C	-5.64	100.99	109.95
1	A	344	GLN	N-CA-C	-5.63	102.94	110.55
1	B	336	ASP	CA-C-N	5.55	126.77	119.84
1	B	336	ASP	C-N-CA	5.55	126.77	119.84
1	C	8	LEU	N-CA-C	5.51	121.98	109.81
1	A	34	GLY	N-CA-C	-5.47	106.98	114.64
1	C	346	ASP	N-CA-C	5.43	117.67	109.41
1	C	10	SER	N-CA-C	5.43	118.00	108.82
1	B	429	ALA	N-CA-C	5.42	117.50	108.99
1	D	143	THR	N-CA-C	-5.34	100.19	108.90
1	B	40	CYS	N-CA-C	5.33	118.26	109.85
1	D	166	ILE	CA-C-N	5.29	126.45	119.84
1	D	166	ILE	C-N-CA	5.29	126.45	119.84
1	A	169	ASN	N-CA-C	5.25	116.68	111.07
1	C	30	ASN	N-CA-C	-5.23	101.36	109.72
1	A	84	ARG	N-CA-C	-5.22	105.59	111.28
1	D	188	THR	N-CA-C	-5.21	101.39	109.72
1	A	225	GLY	CA-C-N	5.20	124.92	119.82
1	A	225	GLY	C-N-CA	5.20	124.92	119.82
1	D	344	GLN	N-CA-C	-5.19	103.55	110.55
1	A	188	THR	N-CA-C	-5.14	101.50	109.72
1	D	495	ILE	CA-C-N	5.13	124.58	119.24
1	D	495	ILE	C-N-CA	5.13	124.58	119.24
1	C	169	ASN	N-CA-C	5.10	117.23	111.11
1	A	483	ARG	N-CA-C	-5.09	107.62	113.88
1	B	10	SER	CA-C-N	5.04	125.32	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	SER	C-N-CA	5.04	125.32	119.92
1	A	345	ILE	N-CA-C	5.02	117.36	111.09
1	C	197	THR	N-CA-C	5.01	115.97	108.76
1	D	30	ASN	N-CA-C	-5.01	103.33	110.59

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	3697	0	3699	224	0
1	B	3689	0	3690	217	0
1	C	3710	0	3710	224	2
1	D	3726	0	3727	230	2
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	C	2	0	0	0	0
4	A	37	0	0	1	0
4	B	53	0	0	3	0
4	C	68	0	0	5	0
4	D	66	0	0	2	0
All	All	15156	0	14874	847	2

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 28.

All (847) 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:D:152:THR:HG22	1:D:492:THR:HB	1.33	1.10
1:B:495:ILE:HG22	1:D:440:LEU:HD13	1.36	1.05
1:A:152:THR:HG22	1:A:492:THR:HB	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ARG:NH1	1:C:341:GLN:HB2	1.74	1.01
1:C:272:LYS:HD3	1:C:423:SER:HB2	1.41	0.99
1:A:2:MET:HG2	1:A:3:ALA:H	1.28	0.98
1:B:152:THR:HG22	1:B:492:THR:HB	1.42	0.98
1:A:329:ARG:HH12	1:A:341:GLN:HB2	1.28	0.96
1:A:442:VAL:HG13	1:A:446:MET:HE3	1.49	0.94
1:C:124:GLY:O	1:C:128:THR:HG23	1.67	0.94
1:A:329:ARG:NH1	1:A:341:GLN:HB2	1.83	0.92
1:B:365:ALA:HB2	1:B:393:MET:HE1	1.52	0.91
1:C:329:ARG:HH12	1:C:341:GLN:HB2	1.27	0.91
1:C:433:THR:HG22	1:C:435:ASP:H	1.33	0.90
1:D:244:THR:HB	1:D:268:GLU:HB3	1.54	0.89
1:C:244:THR:HB	1:C:268:GLU:HB3	1.53	0.89
1:D:6:GLN:N	1:D:6:GLN:HE21	1.71	0.88
1:B:124:GLY:O	1:B:128:THR:HG23	1.74	0.86
1:C:4:SER:HB3	1:C:6:GLN:HE21	1.40	0.86
1:A:433:THR:H	1:A:454:ASN:HD21	1.24	0.86
1:D:124:GLY:O	1:D:128:THR:HG23	1.75	0.86
1:D:433:THR:HG22	1:D:435:ASP:H	1.40	0.84
1:D:457:ASN:HD22	1:D:458:ALA:H	1.25	0.84
1:B:329:ARG:NH1	1:B:341:GLN:HB2	1.94	0.83
1:D:372:LYS:O	1:D:382:GLU:HG2	1.79	0.83
1:A:440:LEU:HD13	1:C:495:ILE:HG22	1.60	0.82
1:C:303:THR:HB	1:C:458:ALA:HB3	1.61	0.82
1:B:29:GLN:HA	1:B:29:GLN:HE21	1.44	0.82
1:B:294:VAL:HG21	1:B:308:ILE:HD11	1.60	0.82
1:C:4:SER:HB3	1:C:6:GLN:NE2	1.95	0.81
1:B:395:ILE:O	1:B:400:ILE:HD11	1.81	0.81
1:D:109:ASN:HD21	1:D:197:THR:HA	1.46	0.80
1:A:196:GLN:H	1:A:196:GLN:HE21	1.28	0.80
1:B:59:ILE:HD13	1:B:221:LEU:HD22	1.62	0.80
1:B:433:THR:HG22	1:B:435:ASP:H	1.46	0.80
1:D:152:THR:CG2	1:D:492:THR:HB	2.11	0.80
1:A:180:ALA:HB3	1:A:181:PRO:HD3	1.64	0.80
1:D:479:GLU:HG3	1:D:483:ARG:HH21	1.46	0.80
1:D:272:LYS:HD3	1:D:423:SER:HB2	1.64	0.79
1:A:124:GLY:O	1:A:128:THR:HG23	1.83	0.78
1:A:294:VAL:HG21	1:A:308:ILE:HD11	1.64	0.78
1:A:400:ILE:HG21	1:A:404:VAL:HB	1.65	0.78
1:D:400:ILE:HG21	1:D:404:VAL:HB	1.65	0.78
1:D:6:GLN:HE21	1:D:6:GLN:CA	1.95	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:PHE:HB3	1:D:329:ARG:HH12	1.48	0.77
1:A:312:GLU:HG2	1:A:409:ARG:HD3	1.67	0.76
1:A:374:LEU:HD12	1:A:380:PHE:HB3	1.66	0.76
1:C:400:ILE:N	1:C:400:ILE:HD12	2.02	0.75
1:A:400:ILE:N	1:A:400:ILE:HD12	2.01	0.75
1:A:331:VAL:HG22	1:A:341:GLN:HB3	1.69	0.75
1:C:8:LEU:H	1:C:9:PRO:HD3	1.52	0.75
1:B:180:ALA:HB3	1:B:181:PRO:HD3	1.69	0.75
1:B:320:LYS:O	1:B:323:VAL:HG22	1.87	0.75
1:B:194:ALA:HB1	1:B:196:GLN:HE21	1.52	0.74
1:D:60:ASP:O	1:D:64:GLN:HG3	1.86	0.74
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.53	0.73
1:A:293:GLY:HA3	1:A:456:TYR:CD2	2.23	0.73
1:C:154:THR:HG22	1:C:490:THR:HB	1.70	0.73
1:C:372:LYS:O	1:C:382:GLU:HG2	1.88	0.73
1:B:329:ARG:HH12	1:B:341:GLN:HB2	1.52	0.73
1:C:293:GLY:O	1:C:304:ALA:HB1	1.88	0.73
1:A:90:LYS:HE2	1:A:211:ALA:O	1.89	0.72
1:B:400:ILE:HD12	1:B:400:ILE:N	2.04	0.72
1:B:173:LEU:HD13	1:B:177:TRP:CH2	2.24	0.72
1:D:457:ASN:HD22	1:D:458:ALA:N	1.86	0.72
1:A:283:LEU:O	1:A:287:VAL:HG23	1.90	0.72
1:D:29:GLN:HE21	1:D:29:GLN:HA	1.53	0.72
1:D:291:HIS:HE1	1:D:329:ARG:HD3	1.54	0.72
1:D:394:ARG:HH11	1:D:394:ARG:HB2	1.55	0.72
1:A:282:ASP:OD1	1:A:285:TYR:HB3	1.89	0.71
1:C:26:ASN:ND2	1:C:215:PRO:HA	2.05	0.71
1:C:280:ASP:OD1	1:C:433:THR:HG23	1.89	0.71
1:D:395:ILE:HD12	1:D:406:GLU:HG2	1.70	0.71
1:D:353:ILE:HD13	1:D:402:GLY:HA3	1.72	0.71
1:B:417:ILE:O	1:B:421:ASN:HB2	1.90	0.71
1:A:44:THR:OG1	1:A:46:GLU:HB3	1.91	0.71
1:A:372:LYS:O	1:A:382:GLU:HG2	1.90	0.71
1:D:413:MET:O	1:D:416:VAL:HG23	1.90	0.71
1:A:272:LYS:HD3	1:A:423:SER:HB2	1.73	0.71
1:B:6:GLN:CD	1:B:6:GLN:H	1.99	0.70
1:C:272:LYS:HD3	1:C:423:SER:CB	2.19	0.70
1:C:21:LYS:HE3	1:C:30:ASN:ND2	2.06	0.70
1:B:56:LYS:HD3	1:B:231:ALA:HB2	1.73	0.70
1:C:21:LYS:HB3	1:C:29:GLN:O	1.91	0.70
1:D:103:ALA:HB2	1:D:122:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:MET:HG2	1:A:3:ALA:N	2.06	0.70
1:A:283:LEU:HD23	1:A:321:ARG:CZ	2.22	0.70
1:C:273:SER:HB3	1:C:305:GLY:N	2.07	0.70
1:D:329:ARG:HG2	1:D:329:ARG:HH11	1.54	0.70
1:B:297:ASN:HD22	1:B:301:CYS:HB3	1.58	0.69
1:D:279:ALA:HA	1:D:314:ILE:HD13	1.74	0.69
1:A:395:ILE:O	1:A:400:ILE:HD11	1.93	0.69
1:D:272:LYS:O	1:D:427:LEU:HD12	1.93	0.68
1:B:6:GLN:CD	1:B:6:GLN:N	2.52	0.68
1:D:2:MET:HE2	1:D:4:SER:H	1.58	0.68
1:C:282:ASP:OD1	1:C:285:TYR:HB3	1.93	0.68
1:B:436:ILE:HA	1:C:436:ILE:HG12	1.76	0.68
1:D:400:ILE:N	1:D:400:ILE:HD12	2.08	0.68
1:C:294:VAL:HG11	1:C:405:GLN:HB3	1.75	0.68
1:C:428:VAL:HG22	1:C:450:THR:HG23	1.75	0.68
1:C:312:GLU:OE2	1:C:411:LYS:HB2	1.93	0.68
1:D:292:GLN:O	1:D:296:PHE:HB2	1.94	0.68
1:A:152:THR:CG2	1:A:492:THR:HB	2.22	0.68
1:B:496:PRO:HG2	1:D:441:MET:HE2	1.77	0.67
1:A:306:SER:O	1:A:308:ILE:HG13	1.93	0.67
1:A:354:LEU:HD23	1:A:357:ILE:HD12	1.75	0.67
1:B:8:LEU:H	1:B:9:PRO:HD2	1.59	0.67
1:A:456:TYR:HD1	1:A:456:TYR:O	1.77	0.67
1:A:196:GLN:O	1:A:197:THR:HG23	1.95	0.67
1:B:436:ILE:HG12	1:C:436:ILE:HA	1.77	0.67
1:C:395:ILE:O	1:C:400:ILE:HD11	1.95	0.66
1:C:180:ALA:HB3	1:C:181:PRO:HD3	1.78	0.66
1:C:194:ALA:HB1	1:C:196:GLN:HE21	1.60	0.66
1:B:413:MET:CE	1:B:438:LYS:HG2	2.26	0.66
1:C:353:ILE:HD13	1:C:402:GLY:HA3	1.78	0.66
1:D:283:LEU:O	1:D:287:VAL:HG23	1.95	0.66
1:C:365:ALA:N	1:C:393:MET:HE1	2.11	0.65
1:D:365:ALA:H	1:D:393:MET:HE1	1.61	0.65
1:C:353:ILE:O	1:C:357:ILE:HG13	1.95	0.65
1:D:59:ILE:HD13	1:D:221:LEU:HD22	1.79	0.65
1:A:77:ARG:HH11	1:D:500:SER:HB2	1.61	0.65
1:A:291:HIS:HE1	1:A:329:ARG:HD2	1.60	0.65
1:A:294:VAL:HG22	1:A:305:GLY:O	1.97	0.65
1:C:317:GLU:O	1:C:321:ARG:HG2	1.97	0.65
1:C:84:ARG:NH1	1:C:184:CYS:O	2.30	0.64
1:A:138:LYS:HD3	1:C:135:TRP:CE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ILE:O	1:B:357:ILE:HG13	1.97	0.64
1:C:255:GLU:HG3	1:D:255:GLU:HG3	1.79	0.64
1:D:264:ARG:NH1	1:D:264:ARG:HG2	2.11	0.64
1:A:247:THR:HA	1:A:269:LEU:HD22	1.79	0.64
1:D:264:ARG:HG2	1:D:264:ARG:HH11	1.60	0.64
1:D:328:ARG:HG2	1:D:328:ARG:HH11	1.62	0.64
1:B:56:LYS:HD3	1:B:231:ALA:CB	2.27	0.64
1:D:12:THR:HG21	1:D:101:THR:HG22	1.79	0.64
1:D:324:GLU:O	1:D:328:ARG:HG3	1.98	0.64
1:B:372:LYS:HG2	1:B:382:GLU:OE2	1.98	0.64
1:C:79:MET:HG2	1:C:83:GLU:HB3	1.80	0.64
1:B:394:ARG:HB2	1:B:394:ARG:NH1	2.13	0.64
1:A:353:ILE:O	1:A:357:ILE:HG13	1.97	0.64
1:C:130:ARG:HG3	1:C:130:ARG:HH11	1.63	0.64
1:D:174:MET:HE3	1:D:174:MET:HA	1.80	0.64
1:A:247:THR:HG22	1:A:269:LEU:HB3	1.81	0.63
1:B:142:MET:HA	1:C:142:MET:HA	1.81	0.63
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.63	0.63
1:A:283:LEU:HD23	1:A:321:ARG:NH2	2.13	0.63
1:B:413:MET:HE2	1:B:438:LYS:HG2	1.81	0.63
1:B:440:LEU:HD13	1:D:495:ILE:HG22	1.80	0.63
1:C:446:MET:HE2	1:C:446:MET:HA	1.81	0.63
1:D:109:ASN:ND2	1:D:197:THR:HA	2.13	0.63
1:A:330:ILE:HG22	1:A:339:THR:HA	1.80	0.63
1:C:457:ASN:HD22	1:C:457:ASN:N	1.97	0.63
1:A:283:LEU:HD23	1:A:321:ARG:NH1	2.14	0.63
1:C:36:VAL:HG11	1:C:50:GLU:HB3	1.81	0.63
1:D:283:LEU:HD21	1:D:317:GLU:HB3	1.80	0.63
1:B:135:TRP:CE2	1:D:138:LYS:HD3	2.33	0.62
1:B:408:LEU:HD12	1:B:408:LEU:H	1.63	0.62
1:A:167:PRO:HD3	1:A:244:THR:O	1.99	0.62
1:A:254:GLN:HG3	1:A:267:LEU:HD11	1.81	0.62
1:D:5:LEU:C	1:D:6:GLN:HE21	2.07	0.62
1:B:7:LEU:HD23	1:B:8:LEU:N	2.15	0.62
1:C:36:VAL:CG1	1:C:50:GLU:HB3	2.28	0.62
1:D:344:GLN:HA	1:D:344:GLN:NE2	2.15	0.62
1:C:99:ARG:HG2	1:C:118:PHE:CE1	2.35	0.62
1:C:394:ARG:HG3	1:C:398:GLU:OE2	1.99	0.62
1:A:2:MET:CG	1:A:3:ALA:H	2.07	0.62
1:B:192:LYS:HG2	1:B:221:LEU:O	1.99	0.62
1:D:195:GLU:HG2	1:D:196:GLN:NE2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:GLU:O	1:C:328:ARG:HG3	1.99	0.61
1:C:280:ASP:CG	1:C:433:THR:HG23	2.25	0.61
1:C:376:ARG:O	1:C:377:LYS:HB2	2.00	0.61
1:A:329:ARG:HH12	1:A:341:GLN:CB	2.09	0.61
1:A:412:THR:OG1	1:A:415:GLU:HB2	2.00	0.61
1:C:248:GLU:H	1:C:248:GLU:CD	2.06	0.61
1:C:319:VAL:O	1:C:323:VAL:HG13	2.00	0.61
1:D:214:PRO:O	1:D:217:VAL:HG23	2.00	0.61
1:A:135:TRP:CE2	1:C:138:LYS:HD3	2.36	0.61
1:B:319:VAL:O	1:B:323:VAL:HG13	2.00	0.61
1:D:275:ASN:ND2	1:D:456:TYR:OH	2.34	0.61
1:A:354:LEU:HA	1:A:357:ILE:HD12	1.82	0.61
1:C:204:MET:O	1:C:208:ILE:HG13	2.00	0.61
1:C:391:ASP:OD2	1:C:419:ARG:HD2	2.01	0.61
1:D:479:GLU:CG	1:D:483:ARG:HH21	2.13	0.61
1:C:59:ILE:HD13	1:C:221:LEU:HD22	1.83	0.60
1:B:349:GLN:O	1:B:353:ILE:HG13	2.01	0.60
1:C:384:THR:HB	1:C:404:VAL:HG22	1.83	0.60
1:C:32:GLU:HG3	1:C:57:VAL:CG1	2.30	0.60
1:D:394:ARG:HH11	1:D:394:ARG:CB	2.13	0.60
1:C:254:GLN:HE21	1:D:254:GLN:HG2	1.66	0.60
1:B:247:THR:HG22	1:B:269:LEU:HB3	1.84	0.60
1:B:365:ALA:CB	1:B:393:MET:HE1	2.30	0.60
1:A:166:ILE:HB	1:A:167:PRO:HD2	1.84	0.60
1:D:2:MET:CE	1:D:4:SER:H	2.13	0.60
1:A:329:ARG:NH1	1:A:341:GLN:OE1	2.34	0.60
1:A:384:THR:HB	1:A:404:VAL:HG22	1.83	0.60
1:D:297:ASN:HD22	1:D:301:CYS:HB3	1.66	0.60
1:C:8:LEU:HD23	1:C:8:LEU:N	2.17	0.59
1:A:408:LEU:HD12	1:A:408:LEU:N	2.17	0.59
1:B:480:PHE:HB2	4:B:727:HOH:O	2.03	0.59
1:A:240:LYS:HG2	1:A:241:ILE:H	1.68	0.59
1:C:26:ASN:ND2	1:C:215:PRO:CA	2.65	0.59
1:D:365:ALA:N	1:D:393:MET:HE1	2.17	0.59
1:A:290:ALA:O	1:A:294:VAL:HG23	2.03	0.59
1:D:353:ILE:O	1:D:357:ILE:HG13	2.03	0.59
1:C:412:THR:OG1	1:C:415:GLU:HB2	2.03	0.59
1:D:344:GLN:HA	1:D:344:GLN:HE21	1.66	0.59
1:A:77:ARG:NH1	1:D:500:SER:HB2	2.17	0.59
1:A:283:LEU:HD21	1:A:317:GLU:HB3	1.83	0.59
1:A:436:ILE:HA	1:D:436:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:MET:HE2	1:C:496:PRO:HG2	1.85	0.59
1:A:442:VAL:CG1	1:A:446:MET:HE3	2.28	0.59
1:D:105:MET:HE1	1:D:203:TYR:CD2	2.38	0.59
1:C:413:MET:HE1	1:C:441:MET:HE3	1.84	0.58
1:D:291:HIS:CE1	1:D:329:ARG:HD3	2.36	0.58
1:D:295:PHE:HB3	1:D:329:ARG:NH1	2.17	0.58
1:A:433:THR:H	1:A:454:ASN:ND2	2.00	0.58
1:D:294:VAL:HG11	1:D:405:GLN:CB	2.33	0.58
1:A:8:LEU:HB3	1:A:9:PRO:CD	2.33	0.58
1:A:109:ASN:ND2	1:A:199:LEU:HG	2.18	0.58
1:C:370:GLY:HA2	1:C:382:GLU:OE2	2.03	0.58
1:D:294:VAL:HG11	1:D:405:GLN:HB3	1.86	0.58
1:A:196:GLN:H	1:A:196:GLN:NE2	1.99	0.58
1:C:6:GLN:C	1:C:7:LEU:HD23	2.27	0.58
1:C:26:ASN:HD22	1:C:215:PRO:CA	2.17	0.58
1:D:408:LEU:N	1:D:408:LEU:HD12	2.19	0.58
1:D:344:GLN:OE1	1:D:403:PRO:HD3	2.03	0.58
1:B:187:ASN:HD21	1:B:485:TYR:HB3	1.68	0.58
1:C:10:SER:HB2	1:C:11:PRO:HD2	1.85	0.58
1:C:71:SER:O	1:C:74:SER:CB	2.51	0.58
1:A:248:GLU:CD	1:A:248:GLU:H	2.12	0.58
1:D:124:GLY:O	1:D:128:THR:CG2	2.51	0.58
1:C:8:LEU:H	1:C:9:PRO:CD	2.16	0.58
1:D:329:ARG:HG2	1:D:329:ARG:NH1	2.18	0.58
1:C:32:GLU:HG3	1:C:57:VAL:HG12	1.85	0.57
1:B:293:GLY:HA3	1:B:456:TYR:CD2	2.40	0.57
1:D:79:MET:HG2	1:D:83:GLU:HB3	1.84	0.57
1:A:240:LYS:HG2	1:A:241:ILE:N	2.18	0.57
1:A:328:ARG:O	1:A:330:ILE:HD12	2.05	0.57
1:C:320:LYS:O	1:C:324:GLU:HG3	2.03	0.57
1:D:173:LEU:HD13	1:D:177:TRP:CH2	2.38	0.57
1:A:258:GLY:HA2	1:A:262:LEU:HD23	1.86	0.57
1:B:264:ARG:HG2	1:B:264:ARG:NH1	2.20	0.57
1:C:4:SER:CB	1:C:6:GLN:HE21	2.15	0.57
1:B:29:GLN:HE21	1:B:29:GLN:CA	2.14	0.57
1:C:174:MET:HE3	1:C:174:MET:HA	1.86	0.57
1:C:294:VAL:HG21	1:C:308:ILE:HD11	1.86	0.57
1:D:8:LEU:HG	1:D:9:PRO:HD2	1.86	0.57
1:A:56:LYS:HD3	1:A:231:ALA:CB	2.35	0.57
1:A:89:ASP:OD1	1:A:130:ARG:HD3	2.05	0.57
1:C:109:ASN:ND2	1:C:199:LEU:HG	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ILE:HB	1:D:167:PRO:HD2	1.87	0.56
1:D:315:TYR:O	1:D:319:VAL:HG23	2.05	0.56
1:B:112:LYS:HG2	1:B:113:PRO:HD2	1.86	0.56
1:B:282:ASP:OD1	1:B:285:TYR:HB3	2.05	0.56
1:C:44:THR:OG1	1:C:46:GLU:HB3	2.06	0.56
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.70	0.56
1:B:21:LYS:HE3	1:B:30:ASN:ND2	2.20	0.56
1:D:12:THR:HG23	1:D:104:THR:HG21	1.87	0.56
1:B:408:LEU:HD12	1:B:408:LEU:N	2.20	0.56
1:C:274:PRO:HD2	1:C:428:VAL:O	2.06	0.56
1:B:146:VAL:HG12	1:B:147:ASP:O	2.05	0.56
1:A:208:ILE:HG23	1:A:213:PHE:CD2	2.41	0.55
1:A:298:GLN:C	1:A:300:GLN:H	2.14	0.55
1:A:36:VAL:CG1	1:A:50:GLU:HB3	2.37	0.55
1:B:248:GLU:CD	1:B:248:GLU:H	2.13	0.55
1:C:400:ILE:HG21	1:C:404:VAL:HB	1.87	0.55
1:C:433:THR:HG22	1:C:434:ASN:N	2.21	0.55
1:A:490:THR:O	1:B:450:THR:HA	2.06	0.55
1:A:426:GLY:O	1:A:427:LEU:HB2	2.06	0.55
1:B:394:ARG:CB	1:B:394:ARG:HH11	2.19	0.55
1:C:89:ASP:OD1	1:C:130:ARG:HD3	2.06	0.55
1:C:166:ILE:CG2	1:C:178:LYS:HD2	2.37	0.55
1:D:320:LYS:O	1:D:323:VAL:HG22	2.06	0.55
1:B:240:LYS:HD3	1:B:241:ILE:N	2.22	0.55
1:C:330:ILE:HD12	1:C:330:ILE:N	2.22	0.55
1:D:400:ILE:CG2	1:D:404:VAL:HB	2.37	0.55
1:A:249:VAL:O	1:A:253:ILE:HG12	2.07	0.55
1:A:301:CYS:SG	1:A:304:ALA:HB2	2.47	0.55
1:D:26:ASN:ND2	1:D:215:PRO:HA	2.21	0.55
1:B:344:GLN:OE1	1:B:403:PRO:HD3	2.07	0.55
1:C:482:LEU:C	1:C:482:LEU:HD12	2.32	0.55
1:C:315:TYR:O	1:C:319:VAL:HG23	2.07	0.55
1:A:262:LEU:HD21	1:B:251:LYS:HG2	1.88	0.54
1:A:343:PRO:HB3	1:A:380:PHE:CE1	2.42	0.54
1:B:70:PHE:CE2	1:B:160:GLY:HA2	2.41	0.54
1:D:328:ARG:O	1:D:330:ILE:HD12	2.08	0.54
1:B:399:GLU:HB3	4:B:732:HOH:O	2.08	0.54
1:D:264:ARG:HH11	1:D:264:ARG:CG	2.20	0.54
1:B:35:ARG:HB2	1:B:35:ARG:NH1	2.22	0.54
1:D:277:ILE:HD13	1:D:318:PHE:CE2	2.43	0.54
1:D:427:LEU:O	1:D:448:ALA:HB1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLU:H	1:A:195:GLU:CD	2.15	0.54
1:A:400:ILE:N	1:A:400:ILE:CD1	2.71	0.54
1:D:169:ASN:H	1:D:169:ASN:HD22	1.55	0.54
1:D:280:ASP:OD1	1:D:433:THR:HG23	2.08	0.54
1:D:301:CYS:SG	1:D:304:ALA:HB2	2.48	0.54
1:D:376:ARG:O	1:D:377:LYS:HB2	2.06	0.54
1:B:232:ILE:HG23	1:B:238:ILE:HD13	1.89	0.54
1:B:89:ASP:OD1	1:B:130:ARG:HD3	2.08	0.54
1:C:455:CYS:O	1:C:456:TYR:HB2	2.07	0.54
1:A:436:ILE:O	1:A:440:LEU:HG	2.06	0.54
1:B:187:ASN:ND2	1:B:485:TYR:HB3	2.23	0.54
1:C:71:SER:O	1:C:74:SER:HB3	2.08	0.54
1:C:247:THR:HA	1:C:269:LEU:HD22	1.89	0.54
1:C:320:LYS:O	1:C:323:VAL:HG22	2.07	0.54
1:C:400:ILE:N	1:C:400:ILE:CD1	2.71	0.54
1:D:410:PHE:CD2	1:D:416:VAL:HG22	2.43	0.54
1:A:315:TYR:O	1:A:319:VAL:HG23	2.08	0.53
1:C:7:LEU:C	1:C:8:LEU:HD23	2.33	0.53
1:D:399:GLU:HG2	1:D:400:ILE:N	2.22	0.53
1:D:400:ILE:HG21	1:D:404:VAL:CB	2.37	0.53
1:A:297:ASN:HD22	1:A:301:CYS:HB3	1.72	0.53
1:B:138:LYS:HD3	1:D:135:TRP:CE2	2.43	0.53
1:A:479:GLU:HG3	1:A:483:ARG:HH21	1.74	0.53
1:D:480:PHE:HA	1:D:483:ARG:NE	2.24	0.53
1:B:109:ASN:ND2	1:B:199:LEU:HG	2.23	0.53
1:B:232:ILE:HG23	1:B:238:ILE:CD1	2.39	0.53
1:B:170:PHE:O	1:B:174:MET:HG2	2.09	0.53
1:C:79:MET:CG	1:C:83:GLU:HB3	2.38	0.53
1:D:221:LEU:HD12	1:D:221:LEU:N	2.24	0.53
1:D:247:THR:HB	1:D:269:LEU:HD13	1.90	0.53
1:A:30:ASN:HD22	1:A:52:GLN:CD	2.17	0.53
1:A:174:MET:HE3	1:A:174:MET:HA	1.90	0.53
1:A:371:GLY:H	1:A:382:GLU:HG3	1.74	0.53
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.44	0.53
1:D:288:GLU:OE1	1:D:325:ARG:CZ	2.57	0.53
1:A:90:LYS:HB2	1:A:90:LYS:NZ	2.24	0.53
1:D:413:MET:HE2	1:D:438:LYS:HG2	1.90	0.53
1:B:194:ALA:HB1	1:B:196:GLN:NE2	2.22	0.52
1:C:353:ILE:CD1	1:C:402:GLY:HA3	2.39	0.52
1:C:413:MET:CE	1:C:438:LYS:HG2	2.39	0.52
1:D:290:ALA:O	1:D:294:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:HH12	1:B:444:SER:HB3	1.73	0.52
1:D:273:SER:O	1:D:305:GLY:HA3	2.08	0.52
1:D:365:ALA:HB2	1:D:393:MET:HE1	1.90	0.52
1:D:394:ARG:HB2	1:D:394:ARG:NH1	2.22	0.52
1:A:320:LYS:O	1:A:323:VAL:HG22	2.09	0.52
1:D:12:THR:HG21	1:D:15:LEU:HD13	1.90	0.52
1:D:178:LYS:HZ3	1:D:244:THR:HG21	1.75	0.52
1:B:90:LYS:HB2	1:B:90:LYS:NZ	2.24	0.52
1:D:6:GLN:CA	1:D:6:GLN:NE2	2.65	0.52
1:A:405:GLN:HG3	1:A:405:GLN:O	2.10	0.52
1:A:433:THR:HG22	1:A:434:ASN:H	1.73	0.52
1:B:442:VAL:HG13	1:B:446:MET:CE	2.40	0.52
1:C:168:TRP:O	1:C:171:PRO:HD3	2.09	0.52
1:D:170:PHE:HB3	1:D:173:LEU:HB2	1.91	0.52
1:A:238:ILE:O	1:A:263:LYS:HE3	2.10	0.52
1:A:280:ASP:OD1	1:A:433:THR:HG22	2.10	0.52
1:B:306:SER:HB3	1:B:406:GLU:OE1	2.09	0.52
1:D:272:LYS:HE3	1:D:307:ARG:NH1	2.25	0.52
1:A:244:THR:HB	1:A:268:GLU:HB2	1.91	0.52
1:A:413:MET:CE	1:A:438:LYS:HG2	2.40	0.52
1:B:323:VAL:O	1:B:327:LYS:HB2	2.09	0.52
1:B:441:MET:HG3	1:D:496:PRO:HG2	1.92	0.51
1:D:290:ALA:HA	1:D:456:TYR:CE2	2.45	0.51
1:D:367:LEU:HD11	1:D:370:GLY:O	2.10	0.51
1:A:264:ARG:NH2	1:A:487:GLU:HB3	2.25	0.51
1:C:169:ASN:HD22	1:C:169:ASN:H	1.58	0.51
1:D:272:LYS:HG3	1:D:427:LEU:HD13	1.92	0.51
1:B:158:PRO:HB3	1:B:185:CYS:O	2.10	0.51
1:B:169:ASN:OD1	1:B:301:CYS:HA	2.10	0.51
1:C:303:THR:HB	1:C:458:ALA:CB	2.37	0.51
1:A:106:GLU:OE2	1:A:171:PRO:HB2	2.10	0.51
1:B:406:GLU:OE1	1:B:406:GLU:N	2.43	0.51
1:B:433:THR:HG22	1:B:435:ASP:N	2.21	0.51
1:C:328:ARG:HH11	1:C:328:ARG:HG2	1.76	0.51
1:C:336:ASP:HB3	1:C:339:THR:HG23	1.93	0.51
1:D:29:GLN:HE21	1:D:29:GLN:CA	2.17	0.51
1:A:365:ALA:HB2	1:A:393:MET:HE1	1.93	0.51
1:B:290:ALA:O	1:B:294:VAL:HG23	2.11	0.51
1:C:453:ILE:HD12	1:D:493:VAL:HG22	1.92	0.51
1:B:166:ILE:HB	1:B:167:PRO:HD2	1.92	0.51
1:B:283:LEU:O	1:B:287:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:GLU:OE1	1:C:106:GLU:HA	2.11	0.51
1:C:438:LYS:O	1:C:442:VAL:HG23	2.11	0.51
1:A:12:THR:O	1:A:15:LEU:HB2	2.11	0.51
1:B:35:ARG:HH11	1:B:35:ARG:CB	2.24	0.51
1:B:77:ARG:HH11	1:B:77:ARG:HB3	1.76	0.51
1:D:275:ASN:ND2	1:D:456:TYR:CZ	2.78	0.51
1:A:312:GLU:HG2	1:A:409:ARG:CD	2.39	0.51
1:B:295:PHE:HB3	1:B:329:ARG:CZ	2.41	0.51
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.46	0.51
1:B:70:PHE:CZ	1:B:160:GLY:HA2	2.46	0.51
1:D:294:VAL:HG22	1:D:305:GLY:O	2.11	0.51
1:A:233:ALA:HA	1:A:241:ILE:HD12	1.92	0.50
1:A:257:ALA:CB	1:A:265:VAL:HG21	2.41	0.50
1:A:319:VAL:HG22	1:A:407:ILE:HG21	1.92	0.50
1:D:332:GLY:C	1:D:339:THR:HG21	2.36	0.50
1:A:17:ILE:HG21	1:A:199:LEU:HD22	1.93	0.50
1:A:109:ASN:HD22	1:A:199:LEU:CG	2.23	0.50
1:A:344:GLN:NE2	1:A:344:GLN:HA	2.26	0.50
1:B:109:ASN:HD22	1:B:199:LEU:CG	2.24	0.50
1:A:105:MET:HE1	1:A:203:TYR:CD1	2.46	0.50
1:B:192:LYS:HD2	1:B:193:PRO:O	2.11	0.50
1:B:324:GLU:O	1:B:328:ARG:HG3	2.11	0.50
1:D:295:PHE:CB	1:D:329:ARG:HH12	2.21	0.50
1:B:214:PRO:O	1:B:217:VAL:HG23	2.12	0.50
1:C:178:LYS:HE3	1:C:242:ALA:HB1	1.94	0.50
1:C:105:MET:HE1	1:C:203:TYR:CD2	2.46	0.50
1:D:275:ASN:ND2	1:D:430:ALA:HB3	2.26	0.50
1:A:11:PRO:C	1:A:12:THR:HG22	2.37	0.50
1:A:36:VAL:HG13	1:A:50:GLU:HB3	1.93	0.50
1:B:400:ILE:HD12	1:B:400:ILE:H	1.75	0.50
1:C:430:ALA:HB2	1:C:456:TYR:CD1	2.46	0.50
1:B:59:ILE:HG13	1:B:231:ALA:HB3	1.93	0.50
1:C:283:LEU:O	1:C:287:VAL:HG23	2.12	0.50
1:B:15:LEU:HD21	1:B:105:MET:HG3	1.93	0.49
1:D:294:VAL:HG13	1:D:306:SER:HA	1.94	0.49
1:A:374:LEU:HD12	1:A:380:PHE:CB	2.40	0.49
1:B:71:SER:O	1:B:72:LEU:C	2.55	0.49
1:B:21:LYS:HB3	1:B:29:GLN:O	2.12	0.49
1:B:433:THR:HG22	1:B:434:ASN:H	1.78	0.49
1:C:254:GLN:HG2	1:D:254:GLN:HE21	1.78	0.49
1:D:173:LEU:HD13	1:D:177:TRP:CZ2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ILE:N	1:B:330:ILE:HD12	2.28	0.49
1:C:292:GLN:HA	1:C:292:GLN:NE2	2.28	0.49
1:C:365:ALA:H	1:C:393:MET:HE1	1.77	0.49
1:A:292:GLN:O	1:A:296:PHE:HB2	2.12	0.49
1:A:401:PHE:CD1	1:A:401:PHE:N	2.79	0.49
1:B:157:GLU:OE1	1:B:489:LYS:HD2	2.13	0.49
1:B:394:ARG:HG3	1:B:398:GLU:OE2	2.12	0.49
1:C:444:SER:HA	1:D:155:ARG:HH12	1.78	0.49
1:D:293:GLY:HA3	1:D:456:TYR:CD1	2.48	0.49
1:B:274:PRO:HB3	1:B:307:ARG:NH1	2.27	0.49
1:C:72:LEU:O	1:C:74:SER:N	2.46	0.49
1:C:295:PHE:HE2	1:C:405:GLN:HE21	1.59	0.49
1:D:11:PRO:O	1:D:12:THR:C	2.56	0.49
1:B:214:PRO:HD2	1:B:217:VAL:HG21	1.95	0.49
1:B:307:ARG:HG3	1:B:307:ARG:HH11	1.77	0.49
1:C:166:ILE:HG22	1:C:178:LYS:HD2	1.95	0.49
1:D:247:THR:HA	1:D:269:LEU:HD22	1.95	0.49
1:D:442:VAL:HG13	1:D:446:MET:CE	2.42	0.49
1:A:427:LEU:HD12	1:A:428:VAL:H	1.77	0.49
1:B:54:ALA:HA	1:B:58:ASP:OD2	2.13	0.49
1:B:285:TYR:CZ	1:B:289:GLN:HG3	2.47	0.49
1:C:408:LEU:HD12	1:C:408:LEU:N	2.27	0.49
1:A:77:ARG:HH11	1:D:500:SER:CB	2.24	0.49
1:A:312:GLU:OE2	1:A:411:LYS:HB2	2.13	0.49
1:A:391:ASP:OD1	1:A:419:ARG:NH1	2.45	0.49
1:C:329:ARG:HH12	1:C:341:GLN:CB	2.13	0.49
1:C:479:GLU:CG	1:C:483:ARG:HH21	2.26	0.49
1:D:36:VAL:CG1	1:D:50:GLU:HB3	2.43	0.48
1:A:246:SER:OG	1:A:249:VAL:HG23	2.13	0.48
1:A:393:MET:O	1:A:397:LYS:HG3	2.13	0.48
1:A:410:PHE:CG	1:A:416:VAL:HG13	2.48	0.48
1:B:7:LEU:HD23	1:B:8:LEU:H	1.78	0.48
1:B:108:LEU:HD13	1:B:108:LEU:O	2.13	0.48
1:C:173:LEU:HD22	1:C:177:TRP:CZ2	2.49	0.48
1:C:478:GLY:N	4:C:712:HOH:O	2.46	0.48
1:C:395:ILE:HG13	1:C:396:ALA:N	2.29	0.48
1:A:29:GLN:HE21	1:A:29:GLN:HA	1.79	0.48
1:A:106:GLU:OE2	1:A:172:LEU:N	2.41	0.48
1:A:138:LYS:HD3	1:C:135:TRP:CD2	2.49	0.48
1:A:294:VAL:HG11	1:A:405:GLN:HB3	1.96	0.48
1:A:400:ILE:CG2	1:A:404:VAL:HB	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LYS:HD3	1:B:423:SER:HB2	1.96	0.48
1:C:55:ASP:O	1:C:56:LYS:C	2.56	0.48
1:C:330:ILE:HD13	1:C:340:GLU:OE2	2.13	0.48
1:D:29:GLN:HA	1:D:29:GLN:NE2	2.26	0.48
1:D:433:THR:HG22	1:D:434:ASN:H	1.78	0.48
1:A:99:ARG:HG2	1:A:118:PHE:CE2	2.48	0.48
1:B:167:PRO:HD3	1:B:244:THR:O	2.12	0.48
1:A:71:SER:O	1:A:74:SER:HB3	2.14	0.48
1:B:166:ILE:CG2	1:B:178:LYS:HD2	2.43	0.48
1:B:365:ALA:HB2	1:B:393:MET:CE	2.36	0.48
1:B:433:THR:HG22	1:B:434:ASN:N	2.29	0.48
1:C:170:PHE:HB3	1:C:173:LEU:HB2	1.96	0.48
1:A:330:ILE:HD12	1:A:330:ILE:N	2.29	0.48
1:C:70:PHE:CE2	1:C:160:GLY:HA2	2.48	0.48
1:C:272:LYS:HG3	1:C:427:LEU:CD1	2.44	0.48
1:C:330:ILE:HG22	1:C:339:THR:HA	1.96	0.48
1:C:394:ARG:HB2	1:C:394:ARG:NH1	2.28	0.48
1:B:113:PRO:HG2	1:B:116:GLN:NE2	2.29	0.48
1:D:32:GLU:HG3	1:D:57:VAL:CG1	2.44	0.48
1:D:90:LYS:HE2	1:D:211:ALA:O	2.13	0.48
1:A:173:LEU:HD22	1:A:177:TRP:CE2	2.49	0.47
1:B:105:MET:HE1	1:B:203:TYR:CG	2.48	0.47
1:B:372:LYS:O	1:B:382:GLU:HG2	2.14	0.47
1:C:169:ASN:H	1:C:169:ASN:ND2	2.12	0.47
1:C:479:GLU:HG3	1:C:483:ARG:HH21	1.78	0.47
1:D:292:GLN:HA	1:D:292:GLN:NE2	2.28	0.47
1:D:395:ILE:O	1:D:400:ILE:HD11	2.14	0.47
1:C:262:LEU:HD13	1:D:269:LEU:HD11	1.95	0.47
1:C:436:ILE:HG22	1:C:440:LEU:HD11	1.97	0.47
1:D:153:PHE:CZ	1:D:491:VAL:HB	2.49	0.47
1:A:158:PRO:HB3	1:A:185:CYS:O	2.14	0.47
1:A:315:TYR:CE1	1:A:407:ILE:HG22	2.49	0.47
1:A:352:LYS:HG2	1:A:401:PHE:HZ	1.79	0.47
1:B:70:PHE:CD1	1:B:77:ARG:HD3	2.49	0.47
1:C:152:THR:HB	1:C:492:THR:HB	1.95	0.47
1:C:435:ASP:OD1	1:C:437:ASN:HB2	2.14	0.47
1:D:169:ASN:H	1:D:169:ASN:ND2	2.13	0.47
1:D:246:SER:HB2	1:D:248:GLU:HG2	1.97	0.47
1:D:347:LYS:HE3	1:D:379:PHE:HE1	1.79	0.47
1:A:439:ALA:CB	1:D:436:ILE:HD11	2.45	0.47
1:B:173:LEU:HD22	1:B:177:TRP:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:HG3	4:A:722:HOH:O	2.14	0.47
1:C:412:THR:O	1:C:415:GLU:HB3	2.13	0.47
1:D:307:ARG:H	1:D:307:ARG:HG2	1.49	0.47
1:A:395:ILE:O	1:A:406:GLU:OE2	2.33	0.47
1:B:208:ILE:HG23	1:B:213:PHE:CD2	2.50	0.47
1:B:236:ILE:CD1	1:B:261:ASN:HB3	2.45	0.47
1:B:394:ARG:HB2	1:B:394:ARG:HH11	1.77	0.47
1:C:254:GLN:HG2	1:D:254:GLN:NE2	2.30	0.47
1:C:344:GLN:OE1	1:C:403:PRO:HD3	2.14	0.47
1:C:357:ILE:HG21	1:C:371:GLY:HA2	1.95	0.47
1:C:409:ARG:O	1:C:419:ARG:NH2	2.48	0.47
1:B:189:VAL:HG12	1:B:190:VAL:N	2.29	0.47
1:B:387:SER:O	1:B:388:ASN:C	2.56	0.47
1:A:44:THR:C	1:A:46:GLU:H	2.22	0.47
1:A:500:SER:O	1:D:77:ARG:NH1	2.46	0.47
1:B:146:VAL:HG21	1:B:152:THR:HG21	1.95	0.47
1:C:272:LYS:HE3	1:C:307:ARG:NH1	2.30	0.47
1:C:356:LEU:HD23	1:C:400:ILE:HG13	1.96	0.47
1:D:26:ASN:ND2	1:D:215:PRO:CA	2.77	0.47
1:D:370:GLY:HA2	1:D:382:GLU:OE2	2.14	0.47
1:D:432:PHE:HA	1:D:454:ASN:OD1	2.14	0.47
1:C:233:ALA:O	1:C:263:LYS:HE2	2.14	0.47
1:C:483:ARG:CZ	4:C:714:HOH:O	2.63	0.47
1:A:123:GLN:O	1:A:127:LYS:HG2	2.15	0.46
1:A:142:MET:HA	1:D:142:MET:HA	1.97	0.46
1:B:204:MET:O	1:B:208:ILE:HG13	2.15	0.46
1:C:247:THR:HG22	1:C:269:LEU:HB3	1.96	0.46
1:C:399:GLU:C	1:C:400:ILE:HD12	2.40	0.46
1:A:4:SER:C	1:A:6:GLN:H	2.23	0.46
1:A:291:HIS:CE1	1:A:329:ARG:HD2	2.46	0.46
1:B:25:ASN:O	1:B:27:GLU:HG2	2.15	0.46
1:B:293:GLY:HA3	1:B:456:TYR:CE2	2.51	0.46
1:C:285:TYR:CZ	1:C:289:GLN:HG3	2.51	0.46
1:D:106:GLU:OE1	1:D:106:GLU:HA	2.15	0.46
1:D:86:ARG:HD3	4:D:719:HOH:O	2.16	0.46
1:A:59:ILE:HD13	1:A:221:LEU:HD22	1.98	0.46
1:C:301:CYS:SG	1:C:304:ALA:HB3	2.55	0.46
1:C:482:LEU:HD12	1:C:482:LEU:O	2.16	0.46
1:D:283:LEU:HD23	1:D:321:ARG:NH2	2.31	0.46
1:C:167:PRO:HD3	1:C:244:THR:O	2.16	0.46
1:A:254:GLN:O	1:A:257:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:LYS:O	1:B:350:TYR:HB3	2.16	0.46
1:B:376:ARG:O	1:B:377:LYS:O	2.33	0.46
1:C:94:LEU:HB3	1:C:207:LEU:HD22	1.98	0.46
1:C:413:MET:C	1:C:415:GLU:N	2.73	0.46
1:D:437:ASN:HB3	1:D:441:MET:HE2	1.96	0.46
1:B:166:ILE:HG22	1:B:178:LYS:HD2	1.97	0.46
1:C:152:THR:HA	1:C:492:THR:HA	1.96	0.46
1:D:247:THR:HG22	1:D:269:LEU:HB3	1.97	0.46
1:D:356:LEU:O	1:D:359:SER:HB3	2.16	0.46
1:A:60:ASP:O	1:A:64:GLN:HG3	2.15	0.46
1:A:451:VAL:HB	1:B:491:VAL:HG22	1.98	0.46
1:B:500:SER:O	1:C:77:ARG:NH1	2.47	0.46
1:A:323:VAL:HG12	1:A:385:VAL:HG11	1.97	0.46
1:C:273:SER:HB3	1:C:305:GLY:H	1.81	0.46
1:A:39:VAL:HG21	1:A:51:VAL:HG23	1.98	0.46
1:B:288:GLU:OE1	1:B:325:ARG:CZ	2.64	0.46
1:D:108:LEU:C	1:D:108:LEU:HD13	2.41	0.46
1:D:387:SER:O	1:D:388:ASN:C	2.59	0.46
1:B:120:ILE:O	1:B:121:ASP:C	2.58	0.45
1:B:315:TYR:O	1:B:319:VAL:HG23	2.16	0.45
1:C:354:LEU:HD23	1:C:357:ILE:HD12	1.98	0.45
1:D:180:ALA:HB3	1:D:181:PRO:HD3	1.97	0.45
1:D:298:GLN:C	1:D:300:GLN:H	2.24	0.45
1:B:62:ALA:HB2	1:B:221:LEU:HD21	1.97	0.45
1:B:301:CYS:SG	1:B:304:ALA:HB2	2.56	0.45
1:C:13:PRO:O	1:C:14:ASN:C	2.58	0.45
1:A:84:ARG:NH1	1:A:184:CYS:O	2.49	0.45
1:B:130:ARG:NH1	1:D:86:ARG:NH1	2.64	0.45
1:B:298:GLN:C	1:B:300:GLN:H	2.25	0.45
1:C:103:ALA:HB2	1:C:122:LEU:HD13	1.98	0.45
1:D:21:LYS:HB3	1:D:29:GLN:O	2.17	0.45
1:D:79:MET:CG	1:D:83:GLU:HB3	2.45	0.45
1:D:413:MET:HE1	1:D:441:MET:CE	2.46	0.45
1:B:12:THR:HG22	1:B:104:THR:OG1	2.17	0.45
1:B:221:LEU:N	1:B:221:LEU:HD12	2.31	0.45
1:B:312:GLU:HG3	1:B:409:ARG:HD3	1.99	0.45
1:C:277:ILE:HD13	1:C:318:PHE:CE2	2.52	0.45
1:C:307:ARG:H	1:C:307:ARG:HG2	1.46	0.45
1:D:290:ALA:HA	1:D:456:TYR:OH	2.16	0.45
1:D:433:THR:HG22	1:D:434:ASN:N	2.31	0.45
1:B:310:VAL:HG21	1:B:318:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:LYS:HB2	1:B:379:PHE:CE1	2.52	0.45
1:B:442:VAL:HG13	1:B:446:MET:HE3	1.99	0.45
1:C:320:LYS:HA	1:C:323:VAL:HG22	1.97	0.45
1:D:295:PHE:CB	1:D:329:ARG:NH1	2.80	0.45
1:D:373:GLY:HA2	1:D:381:ILE:HA	1.97	0.45
1:C:293:GLY:HA3	1:C:456:TYR:HD2	1.81	0.45
1:C:497:GLN:HE21	1:C:499:ASN:HD21	1.63	0.45
1:A:283:LEU:HB3	1:A:321:ARG:HH12	1.81	0.45
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.84	0.45
1:B:109:ASN:OD1	1:B:197:THR:HG22	2.17	0.45
1:C:113:PRO:HG2	1:C:116:GLN:CD	2.41	0.45
1:D:164:GLN:HE22	1:D:179:ILE:HD13	1.82	0.45
1:D:319:VAL:O	1:D:323:VAL:HG13	2.16	0.45
1:C:8:LEU:N	1:C:9:PRO:CD	2.79	0.45
1:C:293:GLY:HA3	1:C:456:TYR:CD2	2.51	0.45
1:D:202:LEU:HD21	1:D:222:PRO:HD3	1.98	0.45
1:A:56:LYS:HD3	1:A:231:ALA:HB1	1.99	0.45
1:A:295:PHE:HE2	1:A:405:GLN:HE21	1.65	0.45
1:B:374:LEU:HB2	4:B:720:HOH:O	2.16	0.45
1:C:391:ASP:OD2	1:C:419:ARG:CD	2.65	0.45
1:A:169:ASN:OD1	1:A:301:CYS:HA	2.17	0.45
1:B:280:ASP:OD2	1:B:433:THR:HG23	2.17	0.45
1:B:402:GLY:O	1:B:404:VAL:N	2.49	0.45
1:B:408:LEU:H	1:B:408:LEU:CD1	2.30	0.45
1:D:14:ASN:N	1:D:14:ASN:HD22	2.14	0.45
1:B:178:LYS:HE3	1:B:242:ALA:HB1	1.99	0.44
1:C:410:PHE:CG	1:C:416:VAL:HG13	2.52	0.44
1:D:274:PRO:HB3	1:D:307:ARG:NH1	2.31	0.44
1:A:489:LYS:NZ	1:B:444:SER:HA	2.31	0.44
1:B:283:LEU:HD13	1:B:314:ILE:HD12	1.99	0.44
1:B:354:LEU:O	1:B:357:ILE:N	2.48	0.44
1:C:367:LEU:HD11	1:C:370:GLY:O	2.17	0.44
1:A:59:ILE:O	1:A:63:VAL:HG23	2.18	0.44
1:A:456:TYR:CD1	1:A:456:TYR:C	2.96	0.44
1:B:247:THR:HA	1:B:269:LEU:HD13	1.99	0.44
1:C:333:SER:O	1:C:339:THR:HG21	2.16	0.44
1:A:10:SER:O	1:A:11:PRO:O	2.36	0.44
1:A:350:TYR:OH	1:A:373:GLY:HA3	2.18	0.44
1:A:352:LYS:CG	1:A:401:PHE:HZ	2.31	0.44
1:B:146:VAL:HG21	1:B:152:THR:CG2	2.48	0.44
1:B:272:LYS:HE3	1:B:307:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ARG:HG2	1:D:118:PHE:CE1	2.52	0.44
1:A:109:ASN:HD22	1:A:199:LEU:HB2	1.81	0.44
1:A:330:ILE:CG2	1:A:339:THR:HA	2.47	0.44
1:A:367:LEU:HD21	1:A:370:GLY:O	2.18	0.44
1:A:370:GLY:HA2	1:A:382:GLU:OE2	2.17	0.44
1:B:293:GLY:O	1:B:456:TYR:HE2	2.00	0.44
1:A:306:SER:HB2	1:A:406:GLU:OE1	2.17	0.44
1:A:324:GLU:O	1:A:328:ARG:HG3	2.16	0.44
1:A:400:ILE:HG21	1:A:404:VAL:CB	2.42	0.44
1:B:6:GLN:H	1:B:6:GLN:NE2	2.16	0.44
1:D:178:LYS:NZ	1:D:244:THR:CG2	2.81	0.44
1:B:55:ASP:O	1:B:56:LYS:C	2.61	0.44
1:B:332:GLY:O	1:B:380:PHE:HE2	2.01	0.44
1:C:146:VAL:CG1	1:C:147:ASP:N	2.81	0.44
1:C:166:ILE:HB	1:C:167:PRO:HD2	1.99	0.44
1:C:384:THR:O	1:C:404:VAL:HA	2.17	0.44
1:D:14:ASN:N	1:D:14:ASN:ND2	2.66	0.44
1:D:25:ASN:O	1:D:27:GLU:HG2	2.18	0.44
1:D:59:ILE:O	1:D:63:VAL:HG23	2.18	0.44
1:A:332:GLY:O	1:A:380:PHE:HE2	2.01	0.44
1:A:428:VAL:HG22	1:A:450:THR:CG2	2.48	0.44
1:B:294:VAL:HG22	1:B:305:GLY:O	2.18	0.44
1:C:300:GLN:HB3	1:C:401:PHE:O	2.18	0.44
1:D:208:ILE:HG23	1:D:213:PHE:CD2	2.53	0.44
1:D:280:ASP:OD1	1:D:433:THR:CG2	2.65	0.44
1:C:234:SER:HB2	4:C:719:HOH:O	2.17	0.44
1:D:111:GLY:O	1:D:343:PRO:HD2	2.18	0.44
1:D:152:THR:HA	1:D:492:THR:HA	1.99	0.44
1:D:273:SER:HA	1:D:428:VAL:O	2.17	0.44
1:D:298:GLN:CD	1:D:298:GLN:N	2.76	0.44
1:D:400:ILE:HD13	1:D:406:GLU:OE1	2.18	0.44
1:A:175:PHE:CD1	1:A:175:PHE:C	2.96	0.43
1:B:8:LEU:H	1:B:9:PRO:CD	2.27	0.43
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.53	0.43
1:B:192:LYS:HD2	1:B:192:LYS:C	2.43	0.43
1:C:71:SER:O	1:C:72:LEU:C	2.60	0.43
1:C:377:LYS:HG2	4:C:752:HOH:O	2.18	0.43
1:A:103:ALA:HB2	1:A:122:LEU:HD13	2.00	0.43
1:A:130:ARG:HG3	1:A:130:ARG:NH1	2.26	0.43
1:A:295:PHE:HE2	1:A:405:GLN:NE2	2.16	0.43
1:B:435:ASP:HA	1:C:434:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:PRO:O	1:D:14:ASN:C	2.61	0.43
1:D:459:LEU:HG	1:D:460:ASN:N	2.32	0.43
1:C:29:GLN:HA	1:C:29:GLN:HE21	1.82	0.43
1:C:248:GLU:CD	1:C:248:GLU:N	2.76	0.43
1:D:112:LYS:HG3	1:D:113:PRO:HD2	1.99	0.43
1:A:496:PRO:HG2	1:C:441:MET:HG3	2.01	0.43
1:B:436:ILE:CA	1:C:436:ILE:HG12	2.45	0.43
1:D:32:GLU:HG3	1:D:57:VAL:HG12	2.00	0.43
1:A:166:ILE:HD13	1:A:166:ILE:H	1.83	0.43
1:B:247:THR:HG22	1:B:269:LEU:HD13	1.99	0.43
1:C:32:GLU:HG3	1:C:57:VAL:HG11	2.00	0.43
1:D:29:GLN:CA	1:D:29:GLN:NE2	2.81	0.43
1:D:274:PRO:CD	1:D:427:LEU:HD11	2.49	0.43
1:D:457:ASN:ND2	1:D:458:ALA:N	2.61	0.43
1:B:12:THR:HG21	1:B:101:THR:HB	2.00	0.43
1:B:109:ASN:HD22	1:B:199:LEU:HG	1.82	0.43
1:B:196:GLN:NE2	1:B:196:GLN:H	2.16	0.43
1:B:236:ILE:HD12	1:B:261:ASN:HB3	2.00	0.43
1:C:267:LEU:CD1	1:D:262:LEU:HD22	2.47	0.43
1:C:302:CYS:C	1:C:304:ALA:H	2.26	0.43
1:D:454:ASN:O	1:D:455:CYS:HB3	2.19	0.43
1:A:70:PHE:CE2	1:A:160:GLY:HA2	2.53	0.43
1:A:273:SER:HB3	1:A:305:GLY:CA	2.49	0.43
1:B:15:LEU:HD12	1:B:16:GLU:N	2.33	0.43
1:C:400:ILE:C	1:C:402:GLY:H	2.26	0.43
1:C:433:THR:HG22	1:C:434:ASN:H	1.84	0.43
1:A:109:ASN:ND2	1:A:199:LEU:CG	2.79	0.43
1:A:356:LEU:HD23	1:A:400:ILE:HG13	2.01	0.43
1:C:7:LEU:C	1:C:8:LEU:CD2	2.92	0.43
1:C:232:ILE:HG23	1:C:238:ILE:CD1	2.49	0.43
1:D:417:ILE:O	1:D:421:ASN:HB2	2.19	0.43
1:A:114:PHE:HD2	1:A:115:LEU:HD23	1.82	0.43
1:B:310:VAL:C	1:B:410:PHE:CE1	2.97	0.43
1:C:125:VAL:HG21	1:C:172:LEU:HG	2.00	0.43
1:C:436:ILE:HG22	1:C:440:LEU:CD1	2.49	0.43
1:D:178:LYS:HZ3	1:D:244:THR:CG2	2.32	0.43
1:D:269:LEU:O	1:D:270:GLY:O	2.36	0.43
1:A:128:THR:HG21	1:A:177:TRP:NE1	2.34	0.43
1:A:432:PHE:HA	1:A:454:ASN:HD22	1.84	0.43
1:B:280:ASP:OD1	1:B:433:THR:HA	2.19	0.43
1:B:421:ASN:ND2	1:B:445:ALA:O	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:PHE:CE2	1:D:160:GLY:HA2	2.54	0.43
1:A:349:GLN:O	1:A:353:ILE:HG13	2.18	0.42
1:C:298:GLN:N	1:C:298:GLN:CD	2.76	0.42
1:A:436:ILE:HA	1:D:436:ILE:CG1	2.49	0.42
1:B:99:ARG:HG2	1:B:118:PHE:CE1	2.53	0.42
1:D:392:ASP:O	1:D:397:LYS:NZ	2.52	0.42
1:B:312:GLU:CG	1:B:409:ARG:HD3	2.48	0.42
1:C:71:SER:O	1:C:74:SER:HB2	2.19	0.42
1:D:178:LYS:NZ	1:D:244:THR:HG21	2.34	0.42
1:A:56:LYS:HD3	1:A:231:ALA:HB2	2.00	0.42
1:A:181:PRO:O	1:A:184:CYS:HB3	2.20	0.42
1:A:198:PRO:O	1:A:202:LEU:HG	2.19	0.42
1:A:277:ILE:HD13	1:A:318:PHE:CE2	2.55	0.42
1:A:435:ASP:OD1	1:A:437:ASN:HB2	2.19	0.42
1:C:94:LEU:HD12	1:C:211:ALA:HB2	2.01	0.42
1:C:221:LEU:N	1:C:221:LEU:HD12	2.33	0.42
1:C:373:GLY:HA2	1:C:381:ILE:HA	2.02	0.42
1:C:421:ASN:O	1:C:422:ASN:C	2.63	0.42
1:D:6:GLN:NE2	1:D:6:GLN:HA	2.34	0.42
1:D:70:PHE:CZ	1:D:160:GLY:HA2	2.54	0.42
1:D:173:LEU:HD23	1:D:173:LEU:HA	1.89	0.42
1:A:169:ASN:HD22	1:A:169:ASN:H	1.67	0.42
1:B:106:GLU:OE2	1:B:171:PRO:HB2	2.20	0.42
1:B:329:ARG:NH1	1:B:341:GLN:OE1	2.52	0.42
1:B:400:ILE:N	1:B:400:ILE:CD1	2.76	0.42
1:B:412:THR:O	1:B:415:GLU:HB3	2.19	0.42
1:C:157:GLU:OE1	1:C:489:LYS:HD2	2.19	0.42
1:C:269:LEU:HD11	1:D:262:LEU:HD13	2.01	0.42
1:D:6:GLN:HE21	1:D:6:GLN:HA	1.82	0.42
1:D:287:VAL:O	1:D:291:HIS:HB2	2.20	0.42
1:D:298:GLN:HG3	1:D:342:GLY:O	2.19	0.42
1:A:298:GLN:C	1:A:300:GLN:N	2.77	0.42
1:B:244:THR:HB	1:B:268:GLU:HB2	2.02	0.42
1:B:264:ARG:HH22	1:B:487:GLU:HB3	1.83	0.42
1:B:333:SER:O	1:B:339:THR:HG21	2.19	0.42
1:C:363:GLU:OE2	1:C:393:MET:HA	2.19	0.42
1:C:431:VAL:HG21	1:C:442:VAL:HG11	2.02	0.42
1:B:293:GLY:HA3	1:B:456:TYR:HD2	1.83	0.42
1:D:459:LEU:HD23	4:D:731:HOH:O	2.20	0.42
1:A:39:VAL:CG2	1:A:51:VAL:HG23	2.50	0.42
1:A:244:THR:HB	1:A:268:GLU:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLY:HA2	1:A:381:ILE:HA	2.01	0.42
1:D:292:GLN:HE21	1:D:292:GLN:CA	2.31	0.42
1:B:144:ILE:HD13	1:C:140:HIS:HD2	1.85	0.42
1:B:269:LEU:O	1:B:270:GLY:O	2.38	0.42
1:B:394:ARG:NH1	1:B:394:ARG:CB	2.78	0.42
1:C:56:LYS:NZ	4:C:719:HOH:O	2.53	0.42
1:C:292:GLN:O	1:C:296:PHE:HB2	2.19	0.42
1:D:220:ILE:C	1:D:221:LEU:HD12	2.45	0.42
1:A:8:LEU:HB3	1:A:9:PRO:HD2	2.01	0.42
1:A:23:PHE:CE1	1:A:26:ASN:HA	2.55	0.42
1:A:323:VAL:HG11	1:A:368:GLU:HB3	2.02	0.42
1:A:329:ARG:HG2	1:A:329:ARG:HH11	1.85	0.42
1:A:479:GLU:CG	1:A:483:ARG:HH21	2.31	0.42
1:B:72:LEU:O	1:B:74:SER:N	2.53	0.42
1:B:109:ASN:HD22	1:B:199:LEU:HD12	1.84	0.42
1:D:11:PRO:HD3	1:D:114:PHE:CD2	2.55	0.42
1:D:11:PRO:HB3	1:D:114:PHE:CD1	2.55	0.42
1:D:300:GLN:HB3	1:D:401:PHE:O	2.20	0.42
1:B:93:ASP:OD1	1:B:130:ARG:NH2	2.47	0.41
1:C:298:GLN:C	1:C:300:GLN:H	2.27	0.41
1:C:457:ASN:N	1:C:457:ASN:ND2	2.66	0.41
1:D:175:PHE:O	1:D:179:ILE:HG12	2.20	0.41
1:D:328:ARG:HH11	1:D:328:ARG:CG	2.31	0.41
1:B:240:LYS:HD3	1:B:240:LYS:C	2.45	0.41
1:C:10:SER:O	1:C:11:PRO:O	2.38	0.41
1:C:283:LEU:HD21	1:C:317:GLU:HB3	2.01	0.41
1:C:306:SER:HB2	1:C:404:VAL:O	2.19	0.41
1:A:292:GLN:NE2	1:A:292:GLN:HA	2.36	0.41
1:A:312:GLU:HG2	1:A:409:ARG:CG	2.50	0.41
1:A:402:GLY:O	1:A:404:VAL:N	2.46	0.41
1:A:427:LEU:HD12	1:A:428:VAL:N	2.35	0.41
1:B:77:ARG:HB3	1:B:77:ARG:NH1	2.36	0.41
1:B:309:PHE:H	1:B:309:PHE:HD1	1.68	0.41
1:C:152:THR:CB	1:C:492:THR:HB	2.50	0.41
1:C:195:GLU:CD	1:C:195:GLU:H	2.29	0.41
1:C:290:ALA:O	1:C:294:VAL:HG23	2.20	0.41
1:D:8:LEU:HD21	1:D:115:LEU:HD11	2.02	0.41
1:D:35:ARG:O	1:D:36:VAL:HG23	2.20	0.41
1:B:285:TYR:CE2	1:B:289:GLN:HG3	2.55	0.41
1:C:303:THR:CB	1:C:458:ALA:HB3	2.41	0.41
1:A:15:LEU:HD21	1:A:105:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ALA:HA	1:A:58:ASP:OD2	2.20	0.41
1:B:294:VAL:O	1:B:294:VAL:HG12	2.19	0.41
1:D:303:THR:CG2	1:D:459:LEU:HB3	2.50	0.41
1:C:413:MET:HG2	1:C:417:ILE:CD1	2.50	0.41
1:D:41:ASN:OD1	1:D:43:ALA:HB3	2.20	0.41
1:D:243:PHE:CD1	1:D:243:PHE:C	2.99	0.41
1:D:353:ILE:CD1	1:D:402:GLY:HA3	2.47	0.41
1:A:15:LEU:HD22	1:A:104:THR:CG2	2.50	0.41
1:A:175:PHE:CE1	1:A:179:ILE:HG13	2.56	0.41
1:A:195:GLU:HB3	1:A:223:GLY:O	2.21	0.41
1:A:399:GLU:HG2	1:A:400:ILE:N	2.36	0.41
1:A:456:TYR:O	1:A:456:TYR:CD1	2.67	0.41
1:B:366:LYS:O	1:B:368:GLU:N	2.54	0.41
1:C:23:PHE:CE1	1:C:26:ASN:HA	2.55	0.41
1:A:113:PRO:HD2	1:A:298:GLN:HE22	1.86	0.41
1:A:282:ASP:OD1	1:A:282:ASP:O	2.39	0.41
1:A:324:GLU:O	1:A:327:LYS:HB2	2.20	0.41
1:B:175:PHE:CD1	1:B:175:PHE:C	2.99	0.41
1:B:283:LEU:HD21	1:B:317:GLU:HB3	2.01	0.41
1:B:309:PHE:N	1:B:309:PHE:CD1	2.88	0.41
1:B:336:ASP:OD1	1:B:336:ASP:C	2.63	0.41
1:B:436:ILE:HG12	1:C:436:ILE:CA	2.50	0.41
1:B:482:LEU:HD12	1:B:482:LEU:C	2.46	0.41
1:C:72:LEU:HD23	1:C:72:LEU:HA	1.79	0.41
1:C:90:LYS:HB2	1:C:90:LYS:NZ	2.36	0.41
1:D:105:MET:HE1	1:D:203:TYR:HD2	1.85	0.41
1:D:295:PHE:HD1	1:D:403:PRO:HA	1.86	0.41
1:D:349:GLN:NE2	1:D:401:PHE:CD2	2.89	0.41
1:A:152:THR:HG22	1:A:492:THR:CB	2.29	0.41
1:A:158:PRO:CD	1:D:500:SER:HB3	2.51	0.41
1:D:153:PHE:CD1	1:D:153:PHE:C	2.99	0.41
1:B:37:PHE:HD1	1:B:53:GLU:HB2	1.85	0.40
1:B:138:LYS:HE3	1:D:135:TRP:CD1	2.56	0.40
1:B:166:ILE:HD12	1:B:191:ILE:HD11	2.02	0.40
1:B:264:ARG:HH11	1:B:264:ARG:CG	2.33	0.40
1:B:279:ALA:HA	1:B:314:ILE:HD13	2.03	0.40
1:B:280:ASP:OD1	1:B:433:THR:HG23	2.21	0.40
1:B:317:GLU:O	1:B:321:ARG:HG2	2.21	0.40
1:A:13:PRO:C	1:A:15:LEU:H	2.28	0.40
1:A:317:GLU:OE1	1:A:321:ARG:NE	2.54	0.40
1:B:244:THR:HA	1:B:268:GLU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:LEU:O	1:C:126:ILE:HG13	2.21	0.40
1:C:279:ALA:HA	1:C:314:ILE:HD13	2.04	0.40
1:A:55:ASP:O	1:A:56:LYS:C	2.63	0.40
1:A:293:GLY:HA3	1:A:456:TYR:CE2	2.54	0.40
1:A:436:ILE:HG13	1:D:434:ASN:C	2.45	0.40
1:C:158:PRO:HB3	1:C:185:CYS:O	2.22	0.40
1:D:14:ASN:HD22	1:D:14:ASN:H	1.67	0.40
1:D:213:PHE:HA	1:D:214:PRO:HD3	1.99	0.40
1:D:264:ARG:NH2	1:D:487:GLU:HB3	2.37	0.40
1:A:274:PRO:HD2	1:A:428:VAL:O	2.21	0.40
1:C:221:LEU:HA	1:C:222:PRO:HD2	1.95	0.40
1:D:249:VAL:O	1:D:253:ILE:HG12	2.22	0.40
1:A:146:VAL:HG12	1:A:147:ASP:O	2.22	0.40
1:A:169:ASN:HD22	1:A:169:ASN:N	2.19	0.40
1:B:72:LEU:O	1:B:73:GLY:C	2.62	0.40
1:B:188:THR:HG22	1:B:217:VAL:HA	2.03	0.40
1:B:283:LEU:HD21	1:B:317:GLU:CB	2.52	0.40
1:B:312:GLU:HG3	1:B:409:ARG:CG	2.51	0.40
1:B:319:VAL:HG22	1:B:407:ILE:HG21	2.03	0.40
1:B:435:ASP:OD1	1:B:437:ASN:HB2	2.21	0.40
1:C:192:LYS:HB3	1:C:192:LYS:HE3	1.88	0.40
1:C:192:LYS:HG2	1:C:221:LEU:O	2.20	0.40
1:C:444:SER:CB	1:D:155:ARG:HH12	2.35	0.40
1:C:492:THR:HG21	1:D:452:TRP:CZ3	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:GLU:OE2	1:D:259:ARG:NH2[2_565]	2.05	0.15
1:C:259:ARG:NH2	1:D:255:GLU:OE2[2_565]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	474/499 (95%)	416 (88%)	48 (10%)	10 (2%)	5	15
1	B	473/499 (95%)	423 (89%)	37 (8%)	13 (3%)	4	10
1	C	476/499 (95%)	419 (88%)	42 (9%)	15 (3%)	3	7
1	D	478/499 (96%)	423 (88%)	48 (10%)	7 (2%)	8	22
All	All	1901/1996 (95%)	1681 (88%)	175 (9%)	45 (2%)	4	12

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	74	SER
1	A	260	SER
1	A	270	GLY
1	B	72	LEU
1	B	270	GLY
1	B	367	LEU
1	C	9	PRO
1	C	11	PRO
1	C	72	LEU
1	C	74	SER
1	D	74	SER
1	B	8	LEU
1	B	74	SER
1	B	316	GLU
1	B	377	LYS
1	C	8	LEU
1	C	270	GLY
1	C	425	PHE
1	D	270	GLY
1	A	425	PHE
1	B	73	GLY
1	C	73	GLY
1	C	401	PHE
1	C	422	ASN
1	C	456	TYR
1	D	425	PHE
1	D	457	ASN
1	A	363	GLU
1	A	377	LYS

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Mol	Chain	Res	Type
1	B	56	LYS
1	B	313	SER
1	B	337	PRO
1	B	425	PHE
1	D	282	ASP
1	D	363	GLU
1	A	415	GLU
1	B	422	ASN
1	C	14	ASN
1	A	427	LEU
1	C	303	THR
1	C	377	LYS
1	C	171	PRO
1	A	378	GLY
1	D	337	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/409 (96%)	364 (92%)	30 (8%)	12	30
1	B	393/409 (96%)	366 (93%)	27 (7%)	14	34
1	C	395/409 (97%)	358 (91%)	37 (9%)	8	21
1	D	397/409 (97%)	361 (91%)	36 (9%)	9	22
All	All	1579/1636 (96%)	1449 (92%)	130 (8%)	10	27

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	8	LEU
1	A	12	THR
1	A	29	GLN
1	A	36	VAL
1	A	46	GLU

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Mol	Chain	Res	Type
1	A	90	LYS
1	A	101	THR
1	A	106	GLU
1	A	115	LEU
1	A	122	LEU
1	A	128	THR
1	A	166	ILE
1	A	192	LYS
1	A	196	GLN
1	A	236	ILE
1	A	248	GLU
1	A	298	GLN
1	A	307	ARG
1	A	355	GLU
1	A	399	GLU
1	A	400	ILE
1	A	416	VAL
1	A	418	GLU
1	A	433	THR
1	A	446	MET
1	A	482	LEU
1	A	490	THR
1	A	492	THR
1	A	496	PRO
1	B	29	GLN
1	B	36	VAL
1	B	46	GLU
1	B	60	ASP
1	B	90	LYS
1	B	101	THR
1	B	122	LEU
1	B	144	ILE
1	B	166	ILE
1	B	179	ILE
1	B	195	GLU
1	B	196	GLN
1	B	244	THR
1	B	248	GLU
1	B	272	LYS
1	B	282	ASP
1	B	298	GLN
1	B	307	ARG

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Mol	Chain	Res	Type
1	B	327	LYS
1	B	399	GLU
1	B	400	ILE
1	B	401	PHE
1	B	416	VAL
1	B	418	GLU
1	B	450	THR
1	B	490	THR
1	B	492	THR
1	C	5	LEU
1	C	6	GLN
1	C	8	LEU
1	C	29	GLN
1	C	30	ASN
1	C	46	GLU
1	C	60	ASP
1	C	75	VAL
1	C	90	LYS
1	C	101	THR
1	C	122	LEU
1	C	142	MET
1	C	152	THR
1	C	166	ILE
1	C	192	LYS
1	C	198	PRO
1	C	236	ILE
1	C	244	THR
1	C	248	GLU
1	C	259	ARG
1	C	263	LYS
1	C	266	THR
1	C	282	ASP
1	C	298	GLN
1	C	307	ARG
1	C	328	ARG
1	C	347	LYS
1	C	355	GLU
1	C	383	PRO
1	C	400	ILE
1	C	401	PHE
1	C	416	VAL
1	C	418	GLU

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Mol	Chain	Res	Type
1	C	450	THR
1	C	457	ASN
1	C	490	THR
1	C	492	THR
1	D	2	MET
1	D	6	GLN
1	D	8	LEU
1	D	12	THR
1	D	46	GLU
1	D	60	ASP
1	D	90	LYS
1	D	113	PRO
1	D	122	LEU
1	D	128	THR
1	D	152	THR
1	D	166	ILE
1	D	167	PRO
1	D	178	LYS
1	D	195	GLU
1	D	196	GLN
1	D	236	ILE
1	D	244	THR
1	D	247	THR
1	D	248	GLU
1	D	254	GLN
1	D	259	ARG
1	D	264	ARG
1	D	282	ASP
1	D	298	GLN
1	D	307	ARG
1	D	394	ARG
1	D	400	ILE
1	D	401	PHE
1	D	416	VAL
1	D	418	GLU
1	D	450	THR
1	D	459	LEU
1	D	482	LEU
1	D	490	THR
1	D	492	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	29	GLN
1	A	30	ASN
1	A	109	ASN
1	A	116	GLN
1	A	123	GLN
1	A	164	GLN
1	A	196	GLN
1	A	291	HIS
1	A	292	GLN
1	A	297	ASN
1	A	422	ASN
1	A	437	ASN
1	A	454	ASN
1	B	25	ASN
1	B	29	GLN
1	B	30	ASN
1	B	116	GLN
1	B	156	HIS
1	B	164	GLN
1	B	196	GLN
1	B	275	ASN
1	B	291	HIS
1	B	292	GLN
1	B	297	ASN
1	B	437	ASN
1	B	497	GLN
1	B	499	ASN
1	C	6	GLN
1	C	14	ASN
1	C	26	ASN
1	C	29	GLN
1	C	30	ASN
1	C	116	GLN
1	C	169	ASN
1	C	196	GLN
1	C	254	GLN
1	C	292	GLN
1	C	358	GLN
1	C	388	ASN
1	C	405	GLN
1	C	422	ASN
1	C	437	ASN

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Mol	Chain	Res	Type
1	C	457	ASN
1	C	497	GLN
1	D	6	GLN
1	D	14	ASN
1	D	29	GLN
1	D	30	ASN
1	D	109	ASN
1	D	156	HIS
1	D	164	GLN
1	D	169	ASN
1	D	196	GLN
1	D	254	GLN
1	D	275	ASN
1	D	291	HIS
1	D	292	GLN
1	D	297	ASN
1	D	457	ASN
1	D	499	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
2	NAD	B	702	-	28,29,48	1.86	7 (25%)	43,45,73	2.17	10 (23%)
2	NAD	C	703	-	28,29,48	2.03	14 (50%)	43,45,73	2.16	10 (23%)
2	NAD	A	701	-	28,29,48	1.96	8 (28%)	43,45,73	2.22	12 (27%)
2	NAD	D	704	-	28,29,48	1.79	7 (25%)	43,45,73	2.17	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	702	-	-	0/16/32/62	0/3/3/5
2	NAD	C	703	-	-	4/16/32/62	0/3/3/5
2	NAD	A	701	-	-	4/16/32/62	0/3/3/5
2	NAD	D	704	-	-	1/16/32/62	0/3/3/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NAD	C4A-N3A	4.85	1.43	1.34
2	B	702	NAD	C4A-N3A	4.27	1.42	1.34
2	D	704	NAD	C4A-N3A	4.15	1.42	1.34
2	A	701	NAD	C5A-N7A	-3.90	1.32	1.39
2	D	704	NAD	C5A-N7A	-3.89	1.32	1.39
2	C	703	NAD	C4A-N3A	3.47	1.40	1.34
2	C	703	NAD	C1B-N9A	3.38	1.55	1.46
2	A	701	NAD	O4B-C1B	3.36	1.49	1.42
2	B	702	NAD	O4B-C1B	3.31	1.49	1.42
2	B	702	NAD	C5A-N7A	-3.31	1.33	1.39
2	A	701	NAD	C1B-N9A	3.27	1.55	1.46
2	C	703	NAD	O4B-C1B	3.27	1.49	1.42
2	B	702	NAD	C1B-N9A	3.22	1.55	1.46
2	C	703	NAD	PA-O3	-3.19	1.56	1.59
2	A	701	NAD	C2A-N1A	3.18	1.39	1.33
2	D	704	NAD	O4B-C1B	3.16	1.49	1.42
2	C	703	NAD	C2A-N3A	2.87	1.39	1.33
2	B	702	NAD	PN-O5D	2.87	1.65	1.54
2	C	703	NAD	C5A-N7A	-2.80	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	704	NAD	C2A-N3A	2.71	1.38	1.33
2	A	701	NAD	C6A-N1A	2.60	1.43	1.35
2	B	702	NAD	C6A-N1A	2.57	1.43	1.35
2	A	701	NAD	C2A-N3A	2.57	1.38	1.33
2	C	703	NAD	C5B-C4B	-2.56	1.43	1.51
2	C	703	NAD	C2A-N1A	2.54	1.38	1.33
2	D	704	NAD	C6A-N1A	2.44	1.42	1.35
2	D	704	NAD	C1B-N9A	2.35	1.52	1.46
2	C	703	NAD	C5A-C4A	2.29	1.43	1.39
2	C	703	NAD	O3B-C3B	2.29	1.48	1.43
2	B	702	NAD	C2A-N1A	2.28	1.38	1.33
2	A	701	NAD	PN-O5D	2.27	1.63	1.54
2	D	704	NAD	PN-O5D	2.26	1.63	1.54
2	C	703	NAD	C6A-N6A	-2.13	1.28	1.34
2	C	703	NAD	C8A-N9A	2.12	1.41	1.37
2	C	703	NAD	C5A-C6A	2.08	1.46	1.41
2	C	703	NAD	PN-O5D	2.01	1.62	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NAD	N3A-C4A-N9A	6.93	138.95	127.17
2	D	704	NAD	C5A-C4A-N3A	-6.83	117.31	126.72
2	C	703	NAD	C5A-C4A-N3A	-6.78	117.38	126.72
2	C	703	NAD	N3A-C4A-N9A	6.72	138.59	127.17
2	A	701	NAD	C5A-C4A-N3A	-6.65	117.56	126.72
2	D	704	NAD	N3A-C4A-N9A	6.64	138.47	127.17
2	B	702	NAD	N3A-C4A-N9A	6.62	138.43	127.17
2	B	702	NAD	C5A-C4A-N3A	-6.61	117.62	126.72
2	A	701	NAD	N3A-C2A-N1A	-5.28	120.58	128.58
2	D	704	NAD	N3A-C2A-N1A	-5.01	121.00	128.58
2	B	702	NAD	N3A-C2A-N1A	-4.99	121.02	128.58
2	C	703	NAD	N3A-C2A-N1A	-4.53	121.73	128.58
2	D	704	NAD	C2A-N3A-C4A	4.15	121.95	111.83
2	B	702	NAD	C2A-N3A-C4A	3.94	121.44	111.83
2	C	703	NAD	C2A-N3A-C4A	3.92	121.41	111.83
2	A	701	NAD	C2A-N3A-C4A	3.66	120.76	111.83
2	A	701	NAD	C6A-C5A-N7A	-3.37	125.59	132.09
2	C	703	NAD	O4B-C1B-N9A	3.17	114.17	108.09
2	B	702	NAD	C6A-C5A-N7A	-3.14	126.04	132.09
2	D	704	NAD	C6A-C5A-N7A	-3.03	126.25	132.09
2	A	701	NAD	C6A-C5A-C4A	2.91	121.16	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	703	NAD	C6A-C5A-N7A	-2.86	126.57	132.09
2	B	702	NAD	C4A-C5A-N7A	2.66	113.62	110.58
2	A	701	NAD	O4B-C1B-N9A	2.64	113.15	108.09
2	D	704	NAD	C6A-C5A-C4A	2.51	120.61	117.18
2	D	704	NAD	O4B-C1B-N9A	2.48	112.86	108.09
2	B	702	NAD	O4B-C1B-N9A	2.45	112.80	108.09
2	A	701	NAD	O2N-PN-O3	2.41	112.72	104.64
2	C	703	NAD	C6A-C5A-C4A	2.38	120.43	117.18
2	B	702	NAD	O4B-C4B-C5B	-2.37	101.73	109.33
2	A	701	NAD	C4A-C5A-N7A	2.34	113.26	110.58
2	B	702	NAD	C6A-C5A-C4A	2.31	120.34	117.18
2	C	703	NAD	O4B-C4B-C5B	-2.30	101.97	109.33
2	A	701	NAD	O4B-C4B-C5B	-2.28	102.04	109.33
2	D	704	NAD	C4A-C5A-N7A	2.23	113.14	110.58
2	D	704	NAD	O4B-C4B-C5B	-2.18	102.34	109.33
2	A	701	NAD	C5A-C4A-N9A	-2.13	103.49	105.81
2	C	703	NAD	C4A-C5A-N7A	2.12	113.00	110.58
2	D	704	NAD	O2N-PN-O1N	2.11	119.04	110.83
2	B	702	NAD	O4B-C4B-C3B	2.03	109.18	105.15
2	C	703	NAD	O4B-C4B-C3B	2.02	109.17	105.15
2	A	701	NAD	O4B-C4B-C3B	2.02	109.16	105.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

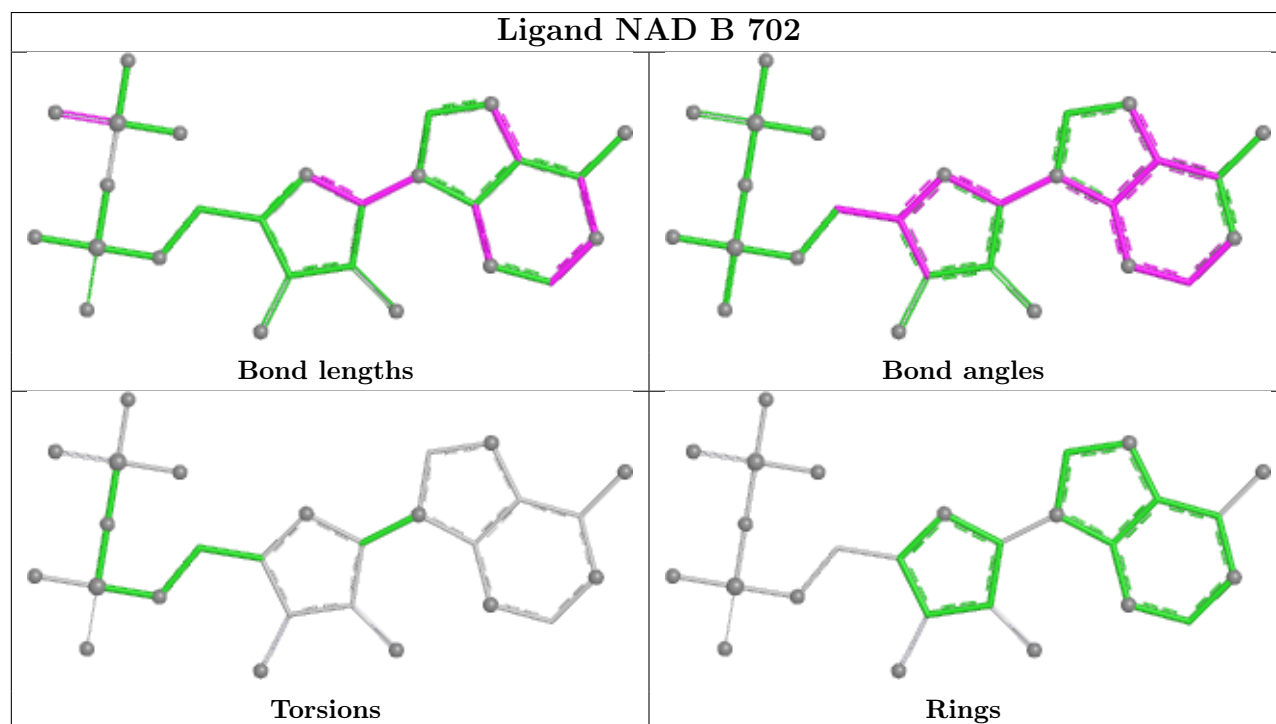
Mol	Chain	Res	Type	Atoms
2	A	701	NAD	PA-O3-PN-O2N
2	C	703	NAD	C5B-O5B-PA-O1A
2	C	703	NAD	C5B-O5B-PA-O2A
2	C	703	NAD	PA-O3-PN-O5D
2	A	701	NAD	PN-O3-PA-O1A
2	A	701	NAD	PA-O3-PN-O5D
2	C	703	NAD	C5B-O5B-PA-O3
2	A	701	NAD	PN-O3-PA-O2A
2	D	704	NAD	C2B-C1B-N9A-C8A

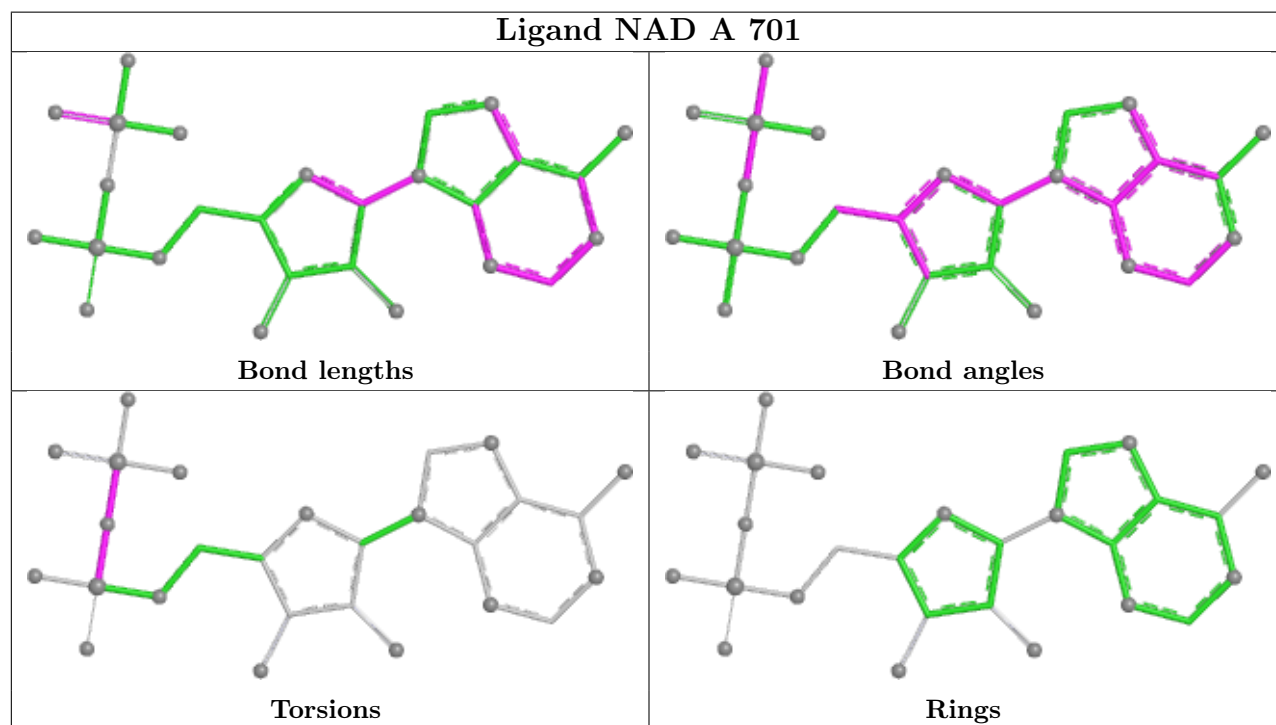
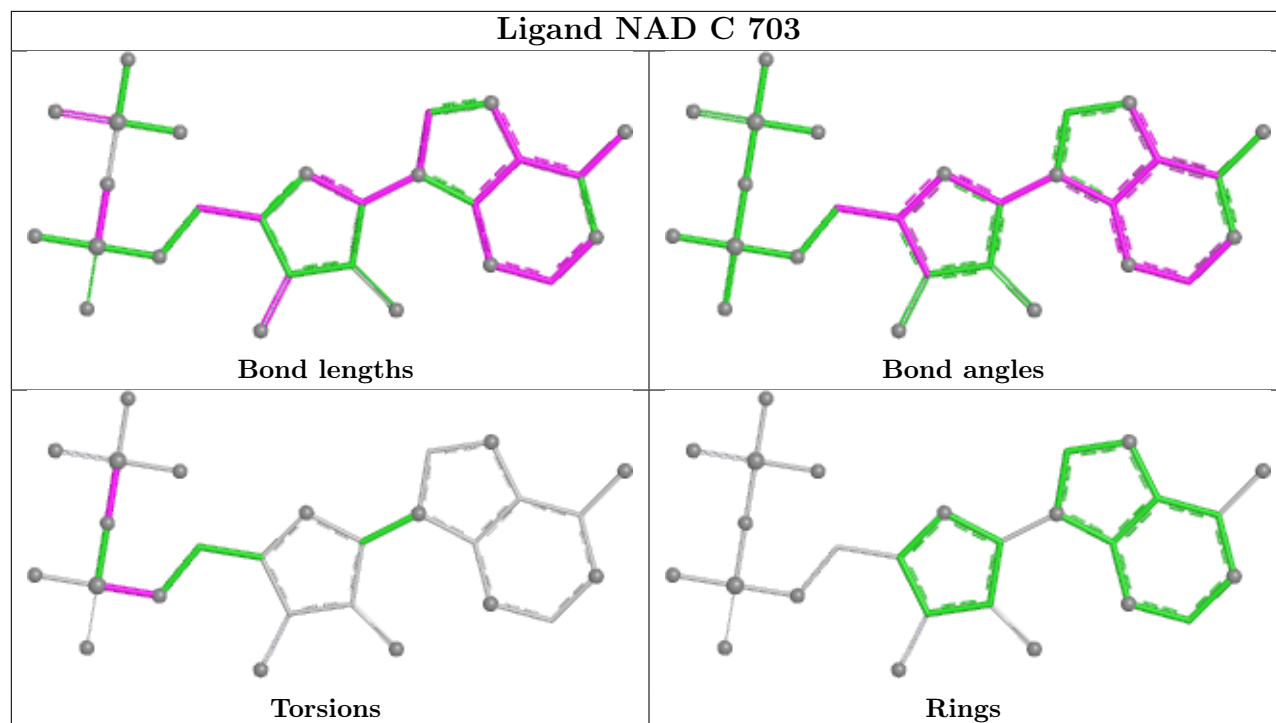
There are no ring outliers.

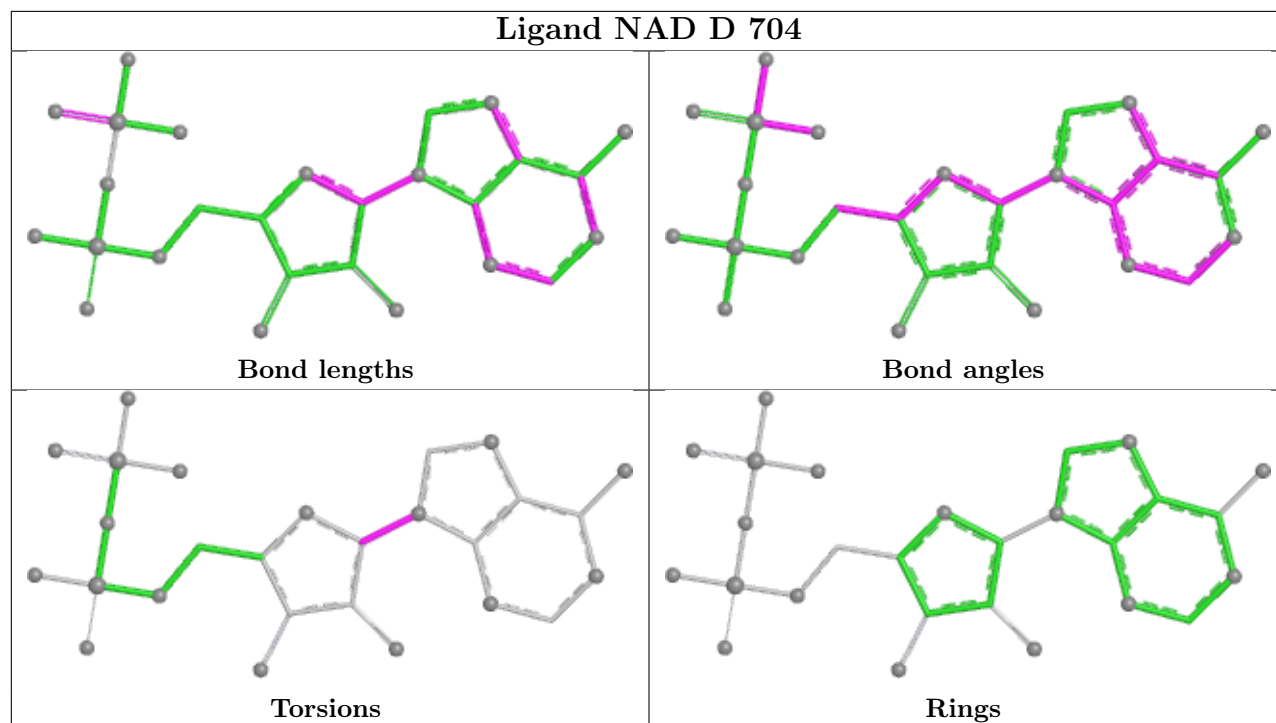
No monomer is involved in short contacts.

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.