



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:50 AM UTC

PDB ID : 6ADH / pdb_00006adh
Title : STRUCTURE OF TRICLINIC TERNARY COMPLEX OF HORSE LIVER
ALCOHOL DEHYDROGENASE AT 2.9 ANGSTROMS RESOLUTION
Authors : Eklund, H.
Deposited on : 1984-01-16
Resolution : 2.90 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

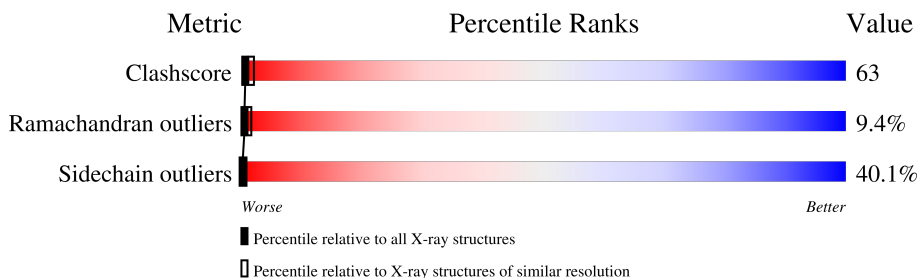
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	374	
1	B	374	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5669 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.

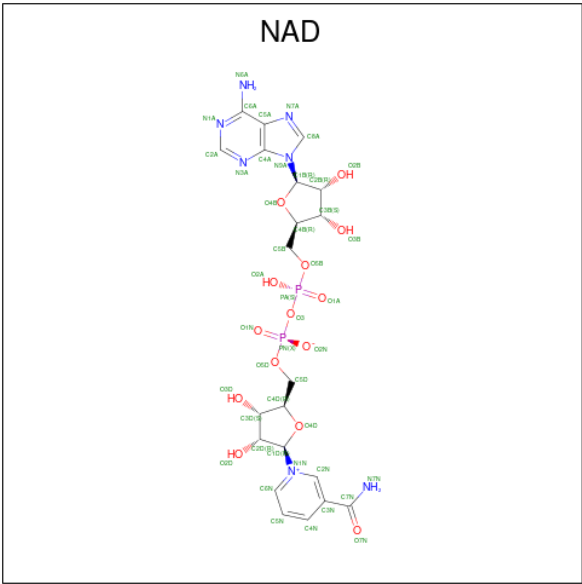
- Molecule 1 is a protein called HOLO-LIVER ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	154	0	0
			2784	1769	472	520	23			
1	B	374	Total	C	N	O	S	151	0	0
			2785	1769	472	521	23			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

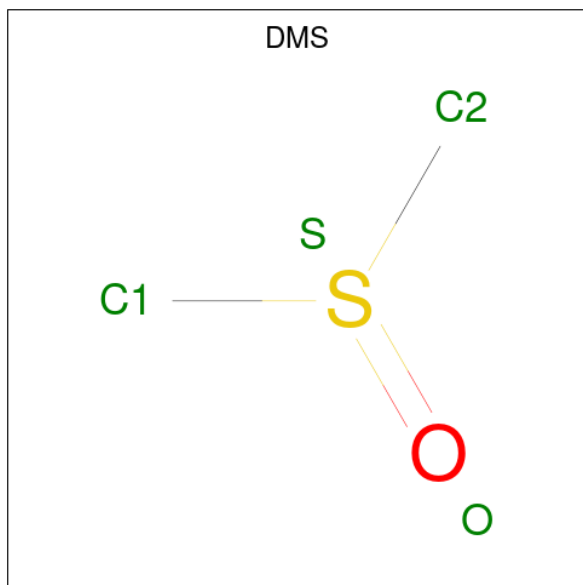
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

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

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

K188	V189	T190	Q191		T194	C195	A196	V197	F198	G199	L200	G201	G202	V203	G204	L205	S206	V207	I208	M209	G210	C211	K212	A213	A214	G215	A216	A217	R218	I219	I220	G221	V222	D223	I224	N225	K226	D227	K228	F229	A230	K231	A232	K233	E234	V235	G236	A237	T238	E239	C240		P243	Q244	D245	Y246	K247	K248	P249
I250	Q251	E252	V253	L254	T255	E256	M257	S258	N259	G260	G261	V262	D263	F264	S265	F266	E267	V268	I269	G270	R271	L272	D273	T274	M275		A278	L279	S280	C281	C282	Q283	E284	A285	Y286	G287	V288	S289	V290	I291	V292	G293	V294	P295	P296	D297		L301	S302	M303	N304	P305	M306	L307	L308	L309	S310	G311	R312
T313	W314	K315		I318	F319		F322	R323	S324	K325	D326	S327	V328	P329	K330	L331	Y332	R333	D334	F335	M336		K339	F340	R341	L342	D343	P344	L345	I346	T347	H348	V349	L350	P351	F352	R353	K354	I355	N356	E357		L361	L362	R363	S364	G365	E366	S367	I368	R369	T370	I371	L372	T373	F374			

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.00Å 44.60Å 94.40Å 104.40° 101.90° 70.70°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5669	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: ZN, DMS, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.29	10/2836 (0.4%)	1.77	77/3834 (2.0%)
1	B	1.50	26/2837 (0.9%)	1.99	113/3834 (2.9%)
All	All	1.40	36/5673 (0.6%)	1.88	190/7668 (2.5%)

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

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

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	CYS	CA-CB	14.02	1.72	1.53
1	B	46	CYS	CA-C	12.98	1.69	1.52
1	B	282	CYS	CA-CB	10.72	1.70	1.53
1	B	160	ILE	CA-C	8.74	1.62	1.52
1	A	83	VAL	N-CA	7.66	1.55	1.46
1	B	161	ASP	N-CA	7.54	1.55	1.46
1	B	128	SER	N-CA	7.09	1.55	1.46
1	B	129	ARG	N-CA	6.99	1.55	1.46
1	B	42	ALA	N-CA	6.64	1.54	1.45
1	B	144	SER	N-CA	6.47	1.54	1.46
1	A	259	ASN	N-CA	6.16	1.54	1.46
1	B	43	THR	N-CA	6.03	1.53	1.46
1	B	63	VAL	N-CA	5.97	1.53	1.46
1	B	216	ALA	N-CA	5.91	1.52	1.45
1	B	62	PRO	C-N	5.87	1.40	1.33
1	B	42	ALA	CA-C	5.81	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	TRP	NE1-CE2	-5.67	1.31	1.37
1	B	100	CYS	CA-CB	5.62	1.62	1.53
1	A	82	THR	CA-C	5.59	1.60	1.52
1	B	154	GLU	N-CA	5.54	1.53	1.46
1	A	314	TRP	NE1-CE2	-5.49	1.31	1.37
1	A	92	LEU	N-CA	5.47	1.53	1.46
1	B	124	GLN	CA-C	5.40	1.60	1.52
1	B	164	SER	CA-C	5.39	1.58	1.52
1	B	127	THR	CA-C	5.39	1.59	1.52
1	B	143	THR	CA-C	5.39	1.59	1.52
1	B	1	SER	C-N	-5.32	1.26	1.33
1	B	153	ASP	CA-C	5.32	1.59	1.52
1	B	314	TRP	NE1-CE2	-5.32	1.31	1.37
1	B	125	ASP	N-CA	5.30	1.53	1.46
1	B	15	TRP	NE1-CE2	-5.21	1.31	1.37
1	A	161	ASP	N-CA	5.19	1.52	1.46
1	B	374	PHE	CA-C	5.12	1.63	1.52
1	A	353	GLU	CA-C	5.12	1.59	1.52
1	A	149	TYR	C-N	-5.09	1.27	1.33
1	A	5	LYS	N-CA	5.05	1.52	1.45

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	CYS	N-CA-CB	26.56	153.26	110.23
1	B	122	THR	O-C-N	13.40	140.41	122.59
1	B	73	VAL	O-C-N	11.99	137.34	122.59
1	A	3	ALA	O-C-N	11.39	137.74	122.59
1	B	292	VAL	O-C-N	10.25	136.24	121.99
1	B	100	CYS	N-CA-CB	-10.12	94.78	110.56
1	B	279	LEU	O-C-N	10.11	132.60	122.09
1	A	367	SER	O-C-N	9.74	135.55	122.59
1	B	127	THR	O-C-N	9.52	134.10	123.25
1	A	118	MET	O-C-N	9.50	132.25	121.32
1	B	127	THR	N-CA-C	9.40	123.36	109.07
1	A	129	ARG	O-C-N	9.35	130.55	121.85
1	B	74	GLU	O-C-N	9.04	128.85	120.71
1	A	1	SER	O-C-N	9.00	137.40	123.00
1	B	282	CYS	N-CA-CB	8.64	123.85	110.46
1	B	46	CYS	N-CA-C	-8.63	95.46	109.96
1	B	54	SER	O-C-N	8.59	130.97	122.03
1	B	58	VAL	O-C-N	8.46	134.35	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	CYS	O-C-N	8.39	132.52	123.03
1	B	10	LYS	O-C-N	8.37	132.72	123.27
1	B	259	ASN	O-C-N	8.35	133.70	122.59
1	A	367	SER	CA-C-N	8.29	136.90	121.97
1	A	367	SER	C-N-CA	8.29	136.90	121.97
1	B	6	VAL	O-C-N	8.26	132.90	122.57
1	A	31	PRO	O-C-N	8.19	132.82	122.91
1	B	292	VAL	CA-C-N	8.19	127.88	120.10
1	B	292	VAL	C-N-CA	8.19	127.88	120.10
1	B	63	VAL	N-CA-C	8.05	118.97	108.35
1	B	238	THR	O-C-N	8.03	131.34	121.95
1	B	350	LEU	CB-CA-C	-7.97	99.51	109.31
1	B	73	VAL	CA-C-N	7.61	132.25	121.98
1	B	73	VAL	C-N-CA	7.61	132.25	121.98
1	A	118	MET	CA-C-N	7.60	128.04	119.83
1	A	118	MET	C-N-CA	7.60	128.04	119.83
1	A	361	LEU	O-C-N	7.40	133.23	122.13
1	B	100	CYS	CB-CA-C	7.38	121.97	109.80
1	B	121	GLY	O-C-N	7.33	131.32	122.60
1	B	127	THR	CA-C-N	7.30	135.48	121.54
1	B	127	THR	C-N-CA	7.30	135.48	121.54
1	B	295	PRO	CB-CA-C	-7.17	102.17	110.92
1	A	195	CYS	CA-CB-SG	7.16	130.87	114.40
1	B	121	GLY	N-CA-C	-7.12	105.66	114.92
1	B	95	PRO	O-C-N	7.07	132.19	122.64
1	B	60	PRO	O-C-N	7.06	131.45	122.91
1	A	45	ILE	O-C-N	7.01	132.33	122.59
1	A	295	PRO	N-CA-C	6.96	119.20	110.70
1	B	134	GLY	O-C-N	6.96	128.58	121.97
1	A	24	GLU	O-C-N	6.93	131.03	122.92
1	A	27	GLU	CB-CA-C	6.90	121.04	110.62
1	B	231	LYS	O-C-N	6.90	129.43	122.12
1	B	23	ILE	O-C-N	6.84	131.12	122.57
1	B	282	CYS	CA-CB-SG	-6.82	98.72	114.40
1	B	58	VAL	N-CA-C	6.74	117.12	106.88
1	A	86	GLY	N-CA-C	-6.73	106.03	115.32
1	B	9	CYS	CA-CB-SG	-6.64	99.13	114.40
1	B	63	VAL	CB-CA-C	-6.58	99.13	111.30
1	A	139	HIS	CA-CB-CG	6.53	120.33	113.80
1	A	194	THR	O-C-N	6.53	131.36	123.13
1	B	30	PRO	O-C-N	6.52	124.31	121.31
1	A	37	ARG	CB-CA-C	6.48	120.73	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	PRO	O-C-N	6.44	130.41	123.01
1	A	296	PRO	O-C-N	6.40	131.28	122.64
1	B	9	CYS	N-CA-CB	6.36	121.08	111.35
1	B	64	ILE	CB-CA-C	-6.36	104.36	111.23
1	B	245	ASP	O-C-N	6.31	130.22	122.34
1	B	170	CYS	N-CA-C	-6.24	105.67	113.28
1	B	122	THR	CA-C-N	6.22	133.42	121.54
1	B	122	THR	C-N-CA	6.22	133.42	121.54
1	A	231	LYS	O-C-N	6.21	130.69	122.43
1	B	98	GLY	N-CA-C	-6.17	106.81	115.32
1	B	118	MET	O-C-N	-6.17	116.24	121.23
1	B	134	GLY	N-CA-C	-6.17	105.07	115.80
1	B	258	SER	N-CA-C	-6.15	105.54	113.16
1	A	295	PRO	O-C-N	6.12	128.69	121.46
1	A	105	HIS	O-C-N	-6.11	113.81	121.70
1	A	108	GLY	O-C-N	6.11	130.64	122.70
1	A	1	SER	CA-C-N	6.10	133.19	121.54
1	A	1	SER	C-N-CA	6.10	133.19	121.54
1	A	3	ALA	CA-C-N	6.10	133.36	121.41
1	A	3	ALA	C-N-CA	6.10	133.36	121.41
1	B	113	LYS	N-CA-C	-6.06	101.39	110.06
1	B	1	SER	CA-C-N	-6.06	113.57	122.78
1	B	1	SER	C-N-CA	-6.06	113.57	122.78
1	A	368	ILE	N-CA-C	6.05	121.93	109.34
1	A	89	VAL	CA-C-N	-6.01	117.62	122.85
1	A	89	VAL	C-N-CA	-6.01	117.62	122.85
1	B	137	ILE	O-C-N	5.99	129.28	122.93
1	B	22	SER	O-C-N	5.97	130.03	123.22
1	B	319	PHE	N-CA-C	-5.96	99.25	108.31
1	A	16	GLU	O-C-N	5.96	130.07	123.52
1	B	279	LEU	CA-C-N	5.95	129.35	120.31
1	B	279	LEU	C-N-CA	5.95	129.35	120.31
1	B	353	GLU	O-C-N	5.95	130.50	122.59
1	B	292	VAL	CA-C-O	-5.93	114.47	120.69
1	B	167	GLU	CB-CA-C	5.88	119.27	109.80
1	B	253	VAL	O-C-N	5.87	129.90	122.57
1	B	25	GLU	N-CA-C	-5.84	101.04	110.32
1	B	119	PRO	O-C-N	5.83	130.29	122.89
1	B	214	ALA	N-CA-C	-5.81	104.78	112.34
1	B	340	PHE	CA-CB-CG	5.76	119.56	113.80
1	A	26	VAL	O-C-N	-5.75	116.66	123.04
1	B	362	LEU	O-C-N	5.74	130.23	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	SER	O-C-N	5.73	128.28	122.09
1	B	101	ARG	CB-CA-C	-5.70	99.07	110.42
1	B	132	CYS	O-C-N	5.69	129.83	122.43
1	A	317	ALA	O-C-N	5.68	129.77	123.52
1	A	345	LEU	O-C-N	5.64	128.65	122.11
1	B	179	GLY	O-C-N	5.64	127.71	122.13
1	B	332	VAL	N-CA-CB	-5.64	104.25	110.51
1	B	98	GLY	O-C-N	5.61	129.55	122.43
1	B	2	THR	N-CA-CB	-5.60	101.60	111.40
1	A	170	CYS	CB-CA-C	5.58	119.36	109.65
1	B	161	ASP	N-CA-C	5.58	122.69	110.80
1	B	214	ALA	O-C-N	5.56	129.56	122.33
1	B	180	TYR	N-CA-CB	-5.55	101.75	110.30
1	B	29	ALA	CA-C-N	5.54	123.70	119.66
1	B	29	ALA	C-N-CA	5.54	123.70	119.66
1	A	37	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	B	43	THR	CB-CA-C	-5.53	99.91	109.86
1	A	133	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	A	129	ARG	N-CA-C	-5.51	105.49	113.21
1	B	348	HIS	CB-CA-C	-5.50	103.14	110.79
1	A	91	PRO	O-C-N	5.50	129.68	123.03
1	B	271	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	363	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	B	231	LYS	N-CA-C	-5.46	104.72	111.33
1	A	170	CYS	N-CA-CB	-5.46	102.40	110.53
1	B	125	ASP	O-C-N	5.45	128.41	122.20
1	A	357	GLU	O-C-N	5.44	129.79	122.49
1	B	58	VAL	CB-CA-C	-5.44	104.36	111.81
1	A	259	ASN	O-C-N	5.42	129.79	122.59
1	B	11	ALA	O-C-N	5.40	129.87	123.33
1	B	75	SER	O-C-N	5.38	129.27	122.65
1	B	169	VAL	N-CA-CB	-5.38	104.95	111.94
1	B	210	GLY	N-CA-C	-5.38	105.89	112.77
1	A	47	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	129	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	B	87	ASP	CB-CA-C	-5.37	102.51	110.62
1	B	218	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	B	120	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	B	369	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A	64	ILE	CB-CA-C	-5.35	106.58	112.68
1	A	218	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	A	312	ARG	NE-CZ-NH2	5.34	124.01	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	GLY	N-CA-C	-5.34	106.68	114.90
1	B	363	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	101	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	A	120	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	B	47	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	A	369	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	180	TYR	O-C-N	5.32	128.61	122.17
1	B	45	ILE	CA-C-N	5.32	129.96	122.09
1	B	45	ILE	C-N-CA	5.32	129.96	122.09
1	A	84	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	274	THR	N-CA-C	-5.28	106.69	113.23
1	B	84	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	B	312	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	297	ASP	O-C-N	5.27	129.59	122.59
1	A	284	GLU	CB-CA-C	-5.24	99.99	110.42
1	B	74	GLU	CB-CA-C	-5.24	104.76	115.28
1	B	129	ARG	NE-CZ-NH2	5.23	123.90	119.20
1	A	354	LYS	O-C-N	5.21	128.68	122.26
1	A	292	VAL	O-C-N	5.21	130.38	122.16
1	A	339	LYS	N-CA-C	-5.20	105.52	111.14
1	A	85	PRO	O-C-N	5.19	129.19	122.91
1	A	168	LYS	O-C-N	5.19	129.49	122.59
1	B	160	ILE	N-CA-CB	-5.19	102.77	112.36
1	B	101	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	357	GLU	N-CA-C	-5.16	107.15	113.50
1	B	37	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	B	251	GLN	O-C-N	5.16	127.45	122.09
1	A	90	ILE	CB-CA-C	5.15	115.37	110.16
1	B	355	ILE	N-CA-C	-5.15	107.80	112.12
1	B	332	VAL	O-C-N	5.13	127.07	121.94
1	B	157	VAL	CB-CA-C	-5.12	102.89	111.29
1	B	27	GLU	O-C-N	5.11	129.57	123.13
1	B	246	TYR	O-C-N	5.11	129.29	123.31
1	B	133	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	205	LEU	N-CA-C	-5.09	107.62	113.88
1	A	148	GLN	N-CA-C	-5.08	107.25	113.50
1	A	9	CYS	CB-CA-C	-5.08	105.20	113.37
1	A	32	LYS	O-C-N	5.07	129.16	123.27
1	B	288	VAL	CB-CA-C	-5.07	103.57	110.77
1	A	335	PHE	O-C-N	5.06	127.92	122.15
1	A	151	VAL	CB-CA-C	-5.06	104.71	110.73
1	A	59	THR	O-C-N	-5.05	118.29	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ILE	O-C-N	5.02	127.69	122.17
1	B	335	PHE	O-C-N	5.02	127.51	122.09
1	A	148	GLN	O-C-N	5.02	129.21	122.49
1	A	170	CYS	O-C-N	5.01	128.99	122.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	46	CYS	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2784	0	2848	338	55
1	B	2785	0	2849	369	59
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	25	4	0
4	A	4	0	6	3	0
4	B	4	0	6	1	0
All	All	5669	0	5760	681	63

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 63.

All (681) 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:132:CYS:HB2	1:A:137:ILE:CD1	1.61	1.29
1:A:255:THR:O	1:A:259:ASN:HA	1.42	1.18
1:B:24:GLU:HG2	1:B:132:CYS:SG	1.86	1.15
1:A:23:ILE:CD1	1:A:353:GLU:HA	1.77	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:CYS:HB2	1:A:137:ILE:HD11	1.22	1.12
1:A:339:LYS:HE2	1:A:339:LYS:HA	1.31	1.11
1:B:59:THR:HG23	1:B:60:PRO:HD2	1.26	1.10
1:B:346:ILE:HD12	1:B:371:ILE:HG12	1.26	1.10
1:B:41:VAL:HG23	1:B:71:GLY:HA2	1.27	1.09
1:B:90:ILE:HG13	1:B:160:ILE:HD13	1.36	1.06
1:B:23:ILE:CD1	1:B:353:GLU:HA	1.86	1.04
1:A:205:LEU:HD22	1:A:235:VAL:HG21	1.41	1.02
1:A:301:LEU:HD21	1:B:303:MET:HE3	1.42	1.02
1:A:243:PRO:HB3	1:A:250:ILE:HG13	1.42	1.01
1:A:23:ILE:HD11	1:A:353:GLU:HA	1.43	1.01
1:A:132:CYS:HB2	1:A:137:ILE:HD12	1.44	1.00
1:A:62:PRO:O	1:A:138:HIS:HB2	1.62	0.98
1:B:255:THR:O	1:B:259:ASN:HA	1.63	0.98
1:B:5:LYS:HA	1:B:30:PRO:HG3	1.46	0.98
1:B:69:ALA:O	1:B:91:PRO:HD2	1.62	0.98
1:A:82:THR:HG23	1:A:154:GLU:OE2	1.64	0.98
1:B:121:GLY:HA3	1:B:138:HIS:HD2	1.23	0.98
1:A:179:GLY:O	1:A:207:VAL:HA	1.64	0.97
1:B:328:VAL:HG22	1:B:329:PRO:HD3	1.46	0.97
1:B:15:TRP:HZ2	1:B:132:CYS:HG	1.02	0.97
1:B:74:GLU:O	1:B:85:PRO:HB3	1.62	0.96
1:B:45:ILE:HG13	1:B:370:THR:HG23	1.45	0.95
1:B:29:ALA:HB1	1:B:30:PRO:HD2	1.46	0.94
1:B:129:ARG:HB3	1:B:139:HIS:CE1	2.02	0.93
1:A:60:PRO:HG2	1:A:121:GLY:HA3	1.49	0.92
1:B:346:ILE:CD1	1:B:371:ILE:HG12	2.00	0.92
1:A:40:MET:HE3	1:A:145:THR:HG22	1.48	0.92
1:B:89:VAL:CG1	1:B:157:VAL:HG23	1.99	0.92
1:B:23:ILE:HD13	1:B:353:GLU:HA	1.52	0.91
1:B:343:ASP:HA	1:B:346:ILE:HG22	1.51	0.91
1:B:349:VAL:HG12	1:B:373:THR:CG2	2.02	0.90
1:A:165:PRO:HB2	1:A:168:LYS:HB2	1.53	0.90
1:A:301:LEU:HD21	1:B:303:MET:CE	2.00	0.90
1:A:124:GLN:HB2	1:A:153:ASP:OD2	1.72	0.90
1:B:88:LYS:HD3	1:B:166:LEU:HD21	1.53	0.90
1:B:327:SER:C	1:B:329:PRO:HD2	1.97	0.90
1:B:232:ALA:O	1:B:237:ALA:HB3	1.70	0.89
1:A:132:CYS:CB	1:A:137:ILE:HD11	2.02	0.89
1:A:179:GLY:HA2	1:A:207:VAL:HG23	1.53	0.89
1:A:208:ILE:HD12	1:A:237:ALA:HB2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HG2	1:B:151:VAL:HG13	1.53	0.88
1:B:59:THR:CG2	1:B:60:PRO:HD2	2.02	0.88
1:A:206:SER:HA	1:A:209:MET:HG2	1.56	0.87
1:A:140:PHE:CE1	1:A:141:LEU:HG	2.10	0.87
1:B:262:VAL:HG13	1:B:263:ASP:H	1.39	0.86
1:B:334:ASP:OD2	1:B:339:LYS:HE3	1.75	0.85
1:B:269:ILE:HD12	1:B:274:THR:HG21	1.58	0.85
1:A:37:ARG:HB3	1:A:151:VAL:HG22	1.58	0.85
1:A:179:GLY:CA	1:A:207:VAL:HG23	2.06	0.85
1:A:208:ILE:CD1	1:A:237:ALA:HB2	2.06	0.85
1:A:304:ASN:ND2	1:A:306:MET:HB2	1.91	0.85
1:B:51:HIS:HB3	1:B:57:LEU:HB2	1.59	0.85
1:B:352:PHE:O	1:B:353:GLU:HB2	1.76	0.85
1:A:190:THR:HG23	1:A:264:PHE:CZ	2.12	0.84
1:B:206:SER:HA	1:B:209:MET:HG3	1.59	0.84
1:A:165:PRO:HG2	1:A:335:PHE:HE1	1.42	0.83
1:B:121:GLY:HA3	1:B:138:HIS:CD2	2.11	0.83
1:B:349:VAL:HG12	1:B:373:THR:HG23	1.60	0.83
1:A:147:SER:HB3	1:A:149:TYR:O	1.77	0.83
1:B:262:VAL:CG1	1:B:263:ASP:H	1.92	0.82
1:B:283:GLN:HG2	1:B:286:TYR:CD2	2.15	0.81
1:A:355:ILE:O	1:A:355:ILE:HG13	1.78	0.81
1:A:5:LYS:HA	1:A:30:PRO:HG3	1.61	0.81
1:B:8:LYS:HG2	1:B:27:GLU:HB2	1.61	0.81
1:B:349:VAL:CG1	1:B:373:THR:CG2	2.59	0.80
1:A:307:LEU:O	1:A:312:ARG:HD2	1.81	0.80
1:B:90:ILE:CG1	1:B:160:ILE:HD13	2.10	0.80
1:B:121:GLY:CA	1:B:138:HIS:HD2	1.94	0.80
1:A:368:ILE:HG13	1:A:369:ARG:N	1.96	0.80
1:B:31:PRO:CG	1:B:75:SER:HB3	2.11	0.80
1:A:206:SER:HA	1:A:209:MET:CG	2.12	0.79
1:A:33:ALA:HA	1:A:78:GLU:H	1.46	0.79
1:A:140:PHE:CD1	1:A:141:LEU:HG	2.17	0.79
1:B:343:ASP:HA	1:B:346:ILE:CG2	2.12	0.79
1:B:203:VAL:HG23	1:B:268:VAL:HG21	1.64	0.78
1:B:97:CYS:HB2	1:B:99:LYS:HB2	1.64	0.78
1:B:345:LEU:O	1:B:368:ILE:HG22	1.83	0.78
1:A:306:MET:HE2	1:A:309:LEU:HD22	1.64	0.78
1:A:174:CYS:O	1:A:178:THR:HG23	1.84	0.77
1:B:179:GLY:HA3	1:B:206:SER:HB2	1.67	0.77
1:B:90:ILE:HG13	1:B:160:ILE:CD1	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:CYS:HB3	1:B:266:PHE:HE1	1.49	0.76
1:A:2:THR:O	1:A:3:ALA:HB2	1.83	0.76
1:A:304:ASN:HD22	1:A:306:MET:H	1.33	0.76
1:A:339:LYS:HA	1:A:339:LYS:CE	2.10	0.76
1:A:13:VAL:HG22	1:A:137:ILE:HG21	1.68	0.75
1:A:232:ALA:O	1:A:235:VAL:HG23	1.86	0.75
1:B:256:GLU:C	1:B:259:ASN:H	1.94	0.75
1:A:315:LYS:HG2	1:B:313:THR:HB	1.67	0.75
1:A:231:LYS:O	1:A:235:VAL:HG22	1.87	0.74
1:B:89:VAL:HG13	1:B:157:VAL:HG23	1.70	0.74
1:B:16:GLU:HB3	1:B:19:LYS:HG2	1.69	0.74
1:A:272:LEU:HD12	1:B:305:PRO:HG3	1.68	0.74
1:B:262:VAL:CG1	1:B:263:ASP:N	2.50	0.74
1:A:32:LYS:HB2	1:A:129:ARG:NH1	2.02	0.73
1:B:45:ILE:HG13	1:B:370:THR:CG2	2.17	0.73
1:B:171:LEU:HD11	1:B:369:ARG:HG2	1.69	0.73
1:B:225:ASN:HD22	1:B:228:LYS:HD2	1.52	0.73
1:A:253:VAL:HG12	1:A:257:MET:HE3	1.71	0.73
1:B:59:THR:HG23	1:B:60:PRO:CD	2.13	0.73
1:B:186:VAL:CG2	1:B:290:VAL:HG11	2.18	0.73
1:B:29:ALA:HB1	1:B:30:PRO:CD	2.19	0.73
1:B:31:PRO:HG2	1:B:75:SER:HB3	1.70	0.72
1:A:4:GLY:O	1:A:30:PRO:HB3	1.89	0.72
1:A:17:GLU:O	1:A:18:LYS:HB2	1.88	0.72
1:B:89:VAL:HG11	1:B:157:VAL:HG23	1.70	0.72
1:B:218:ARG:HH21	1:B:220:ILE:HD11	1.54	0.72
1:A:96:GLN:HG3	1:A:97:CYS:H	1.53	0.72
1:A:337:ALA:C	1:A:338:LYS:HG2	2.13	0.72
1:B:271:ARG:HB3	1:B:274:THR:HB	1.71	0.72
1:B:84:ARG:O	1:B:87:ASP:HB2	1.88	0.71
1:A:183:ALA:O	1:A:189:VAL:HG23	1.89	0.71
1:B:232:ALA:O	1:B:237:ALA:CB	2.37	0.71
1:B:157:VAL:HG22	1:B:158:ALA:N	2.05	0.71
1:A:35:GLU:CD	1:A:123:MET:HE2	2.14	0.71
1:A:301:LEU:CD2	1:B:303:MET:HE3	2.20	0.71
1:B:268:VAL:O	1:B:268:VAL:CG2	2.37	0.71
1:B:129:ARG:HG2	1:B:151:VAL:CG1	2.21	0.71
1:A:13:VAL:HG23	1:A:64:ILE:HD13	1.71	0.70
1:B:132:CYS:H	1:B:137:ILE:HG12	1.55	0.70
1:B:190:THR:HG22	1:B:191:GLN:N	2.05	0.70
1:B:8:LYS:CG	1:B:27:GLU:HB2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:VAL:O	1:A:169:VAL:HG13	1.92	0.70
1:B:328:VAL:N	1:B:329:PRO:HD2	2.07	0.70
1:B:165:PRO:HB2	1:B:168:LYS:HB2	1.73	0.69
1:A:232:ALA:HA	1:A:235:VAL:CG2	2.22	0.69
1:B:268:VAL:O	1:B:268:VAL:HG22	1.93	0.69
1:B:122:THR:OG1	1:B:123:MET:N	2.18	0.69
1:A:35:GLU:HG2	1:A:123:MET:HE2	1.74	0.69
1:A:160:ILE:HG12	1:A:161:ASP:N	2.06	0.69
1:A:251:GLN:HG3	1:A:277:THR:HG23	1.74	0.69
1:A:190:THR:HG23	1:A:264:PHE:HZ	1.57	0.69
1:A:205:LEU:O	1:A:209:MET:HG2	1.93	0.69
1:B:131:THR:HG23	1:B:131:THR:O	1.91	0.69
1:A:243:PRO:HB3	1:A:250:ILE:CG1	2.21	0.68
1:A:363:ARG:HG3	1:A:364:SER:N	2.08	0.68
1:A:13:VAL:HG21	1:A:137:ILE:HD13	1.74	0.68
1:B:275:MET:HE1	1:B:295:PRO:HG3	1.74	0.68
1:A:37:ARG:CB	1:A:151:VAL:HG22	2.23	0.68
1:B:169:VAL:CG1	1:B:332:VAL:HG22	2.24	0.68
1:A:255:THR:CG2	1:A:281:CYS:HA	2.24	0.68
1:A:68:GLU:HG3	1:A:174:CYS:HB3	1.74	0.67
1:A:350:LEU:HB2	1:A:372:LEU:HD12	1.75	0.67
1:A:98:GLY:O	1:A:99:LYS:HB2	1.94	0.67
1:A:179:GLY:O	1:A:207:VAL:CA	2.42	0.67
1:B:64:ILE:HB	1:B:144:SER:HB3	1.77	0.67
1:A:187:ALA:O	1:A:188:LYS:HB2	1.93	0.67
1:A:205:LEU:CD2	1:A:235:VAL:HG21	2.22	0.67
1:B:160:ILE:HG23	1:B:332:VAL:HG11	1.75	0.67
1:B:51:HIS:HB3	1:B:57:LEU:CB	2.25	0.66
1:A:255:THR:O	1:A:259:ASN:CA	2.33	0.66
1:A:296:PRO:HB2	1:A:299:GLN:NE2	2.09	0.66
1:B:15:TRP:HZ2	1:B:132:CYS:SG	2.13	0.66
1:B:121:GLY:C	1:B:122:THR:HG23	2.20	0.66
1:B:157:VAL:CG2	1:B:158:ALA:N	2.59	0.66
1:B:301:LEU:CD1	1:B:301:LEU:O	2.44	0.66
1:B:343:ASP:C	1:B:345:LEU:H	2.03	0.66
1:B:225:ASN:ND2	1:B:228:LYS:HD2	2.11	0.66
1:A:161:ASP:O	1:A:162:ALA:HB2	1.96	0.66
1:A:176:PHE:HE2	1:A:209:MET:HE2	1.59	0.66
1:B:73:VAL:HG12	1:B:75:SER:O	1.96	0.65
1:B:88:LYS:CD	1:B:166:LEU:HD21	2.25	0.65
1:A:350:LEU:HD22	1:A:370:THR:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:HIS:HB2	1:A:370:THR:HG23	1.78	0.65
1:B:59:THR:CG2	1:B:60:PRO:CD	2.70	0.65
1:B:87:ASP:O	1:B:89:VAL:HG23	1.97	0.65
1:A:168:LYS:HG2	1:A:335:PHE:HZ	1.61	0.65
1:A:97:CYS:SG	1:A:98:GLY:N	2.70	0.65
1:A:335:PHE:CD2	1:A:342:LEU:HD22	2.32	0.65
1:B:243:PRO:HA	1:B:250:ILE:HG12	1.79	0.65
1:B:355:ILE:C	1:B:357:GLU:H	2.05	0.64
1:A:57:LEU:HD12	1:A:58:VAL:N	2.12	0.64
1:A:206:SER:CA	1:A:209:MET:HG2	2.27	0.64
1:B:169:VAL:HG13	1:B:332:VAL:HG22	1.78	0.64
1:B:328:VAL:N	1:B:329:PRO:CD	2.60	0.64
1:A:161:ASP:HB3	1:A:164:SER:OG	1.97	0.64
1:A:190:THR:HG23	1:A:264:PHE:CE1	2.32	0.64
1:A:251:GLN:CG	1:A:277:THR:HG23	2.28	0.64
1:B:203:VAL:HG23	1:B:268:VAL:CG2	2.27	0.64
1:B:301:LEU:CD1	1:B:301:LEU:C	2.70	0.64
1:B:39:LYS:HB2	1:B:149:TYR:CE1	2.32	0.64
1:A:305:PRO:HB2	1:B:275:MET:HE2	1.79	0.64
1:A:343:ASP:N	1:A:344:PRO:HD2	2.13	0.64
1:B:283:GLN:HG3	1:B:285:ALA:H	1.63	0.64
1:B:91:PRO:HB2	1:B:143:THR:HG22	1.80	0.63
1:A:90:ILE:HD11	1:A:328:VAL:HG13	1.80	0.63
1:B:41:VAL:HG21	1:B:166:LEU:CD1	2.28	0.63
1:A:131:THR:HA	1:A:136:PRO:HA	1.80	0.63
1:B:102:VAL:HG11	1:B:110:PHE:O	1.98	0.63
1:B:169:VAL:HG13	1:B:332:VAL:CG2	2.28	0.63
1:B:179:GLY:O	1:B:207:VAL:HG22	1.97	0.63
1:A:161:ASP:O	1:A:162:ALA:CB	2.47	0.63
1:A:335:PHE:HE2	1:A:342:LEU:HB2	1.62	0.63
1:B:31:PRO:HG3	1:B:75:SER:HB3	1.80	0.63
1:A:205:LEU:HA	1:A:208:ILE:HG23	1.81	0.63
1:B:41:VAL:HG21	1:B:166:LEU:HD12	1.79	0.63
1:A:76:ILE:HD13	1:A:85:PRO:HD3	1.81	0.63
1:A:146:PHE:O	1:A:352:PHE:CZ	2.51	0.63
1:A:204:GLY:O	1:A:208:ILE:CG2	2.46	0.63
1:B:63:VAL:HG22	1:B:64:ILE:C	2.23	0.63
1:B:177:SER:O	1:B:181:GLY:N	2.31	0.63
1:A:205:LEU:HD22	1:A:235:VAL:CG2	2.24	0.62
1:A:230:ALA:C	1:A:232:ALA:H	2.06	0.62
1:B:334:ASP:OD2	1:B:339:LYS:CE	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:O	1:B:369:ARG:HB2	1.97	0.62
1:B:190:THR:CG2	1:B:191:GLN:N	2.63	0.62
1:A:35:GLU:CG	1:A:123:MET:HE2	2.29	0.62
1:A:165:PRO:HG2	1:A:335:PHE:CE1	2.29	0.62
1:B:129:ARG:HB3	1:B:139:HIS:NE2	2.14	0.62
1:B:327:SER:C	1:B:329:PRO:CD	2.72	0.62
1:A:57:LEU:HD12	1:A:57:LEU:C	2.25	0.61
1:B:131:THR:O	1:B:131:THR:CG2	2.49	0.61
1:A:160:ILE:HG12	1:A:161:ASP:H	1.65	0.61
1:A:303:MET:CG	1:A:304:ASN:N	2.63	0.61
1:B:122:THR:OG1	1:B:123:MET:HG2	2.00	0.61
1:B:328:VAL:CG2	1:B:329:PRO:HD3	2.27	0.61
1:A:60:PRO:HB2	1:A:138:HIS:CE1	2.35	0.61
1:A:123:MET:HG3	1:A:124:GLN:H	1.64	0.61
1:A:347:THR:HB	1:A:348:HIS:ND1	2.15	0.61
1:B:213:ALA:C	1:B:215:GLY:N	2.54	0.61
1:A:255:THR:HG23	1:A:281:CYS:HA	1.83	0.61
1:A:96:GLN:HG3	1:A:97:CYS:N	2.16	0.61
1:B:41:VAL:CG2	1:B:71:GLY:HA2	2.18	0.61
1:B:88:LYS:HD3	1:B:166:LEU:CD2	2.29	0.61
1:B:46:CYS:HB3	1:B:369:ARG:NH2	2.17	0.60
1:B:70:ALA:HB1	1:B:166:LEU:HD22	1.83	0.60
1:A:335:PHE:CE2	1:A:342:LEU:HB2	2.37	0.60
1:B:166:LEU:C	1:B:167:GLU:HG3	2.26	0.60
1:B:249:PRO:O	1:B:252:GLU:HG3	2.01	0.60
1:B:89:VAL:HA	1:B:158:ALA:O	2.00	0.60
1:B:158:ALA:O	1:B:160:ILE:HD12	2.01	0.60
1:B:343:ASP:CA	1:B:346:ILE:HG22	2.30	0.60
1:A:48:SER:HA	1:A:51:HIS:CD2	2.36	0.60
1:A:200:LEU:HD12	1:A:223:ASP:HB2	1.82	0.60
1:B:206:SER:CA	1:B:209:MET:HG3	2.30	0.60
1:A:350:LEU:HD13	1:A:370:THR:HG23	1.84	0.60
1:B:129:ARG:HB3	1:B:139:HIS:HE1	1.58	0.60
1:B:348:HIS:O	1:B:370:THR:HA	2.02	0.60
1:B:195:CYS:HA	1:B:264:PHE:O	2.02	0.59
1:A:284:GLU:O	1:A:310:SER:HB2	2.01	0.59
1:B:271:ARG:HB3	1:B:274:THR:CB	2.32	0.59
1:A:117:SER:O	1:A:118:MET:HB3	2.02	0.59
1:A:60:PRO:HG2	1:A:121:GLY:CA	2.28	0.59
1:A:92:LEU:CD1	1:A:325:LYS:HG2	2.32	0.59
1:A:140:PHE:O	1:A:142:GLY:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:N	1:A:329:PRO:HD2	2.18	0.59
1:B:180:TYR:O	1:B:184:VAL:HG23	2.02	0.59
1:A:10:LYS:HD3	1:A:23:ILE:HG22	1.84	0.59
1:B:334:ASP:O	1:B:339:LYS:HB2	2.02	0.59
1:A:37:ARG:HA	1:A:150:THR:O	2.03	0.59
1:A:40:MET:CE	1:A:145:THR:HG22	2.27	0.59
1:A:220:ILE:HG22	1:A:241:VAL:HG12	1.85	0.59
1:B:132:CYS:HB3	1:B:137:ILE:HG13	1.83	0.59
1:A:96:GLN:CG	1:A:97:CYS:N	2.65	0.59
1:A:355:ILE:HB	1:A:372:LEU:CD2	2.32	0.59
1:A:39:LYS:N	1:A:72:ILE:O	2.36	0.59
1:A:208:ILE:HD11	1:A:235:VAL:HG23	1.85	0.59
1:B:272:LEU:HG	1:B:301:LEU:HB3	1.84	0.59
1:B:91:PRO:HB2	1:B:143:THR:CG2	2.33	0.58
1:B:172:ILE:O	1:B:172:ILE:HG22	2.01	0.58
1:A:306:MET:HE2	1:A:309:LEU:CD2	2.33	0.58
1:B:165:PRO:C	1:B:167:GLU:H	2.11	0.58
1:B:132:CYS:HB3	1:B:137:ILE:CG1	2.32	0.58
1:B:194:THR:HG23	1:B:218:ARG:HB3	1.86	0.58
1:A:352:PHE:CD2	1:A:374:PHE:CE2	2.91	0.58
1:A:13:VAL:CG2	1:A:64:ILE:HD13	2.33	0.58
1:A:154:GLU:O	1:A:157:VAL:HG12	2.03	0.58
1:A:178:THR:HG22	1:A:319:PHE:CD1	2.39	0.58
1:A:13:VAL:HG23	1:A:64:ILE:CD1	2.33	0.58
1:A:251:GLN:HG3	1:A:277:THR:CG2	2.33	0.58
1:A:305:PRO:CB	1:B:275:MET:HE2	2.34	0.58
1:B:96:GLN:HG3	1:B:325:LYS:H	1.69	0.58
1:A:2:THR:O	1:A:3:ALA:CB	2.51	0.58
1:B:243:PRO:HB3	1:B:250:ILE:HG13	1.85	0.58
1:A:77:GLY:H	1:A:80:VAL:HG21	1.69	0.58
1:A:84:ARG:O	1:A:87:ASP:HB2	2.04	0.58
1:B:62:PRO:O	1:B:138:HIS:HB2	2.04	0.58
1:A:32:LYS:HB2	1:A:129:ARG:HH12	1.65	0.58
1:A:146:PHE:O	1:A:352:PHE:HZ	1.87	0.58
1:A:129:ARG:HG2	1:A:151:VAL:CG2	2.33	0.57
1:A:262:VAL:HG23	1:A:264:PHE:O	2.03	0.57
1:B:301:LEU:O	1:B:301:LEU:HD13	2.05	0.57
1:A:47:ARG:C	1:A:49:ASP:H	2.11	0.57
1:A:178:THR:HG22	1:A:319:PHE:HD1	1.69	0.57
1:A:309:LEU:HD23	1:B:318:ILE:HD11	1.87	0.57
1:B:249:PRO:HG2	1:B:252:GLU:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ALA:O	1:A:91:PRO:HD2	2.03	0.57
1:A:343:ASP:N	1:A:344:PRO:CD	2.67	0.57
1:B:26:VAL:CG2	1:B:132:CYS:HB2	2.34	0.57
1:B:72:ILE:HG22	1:B:87:ASP:N	2.20	0.57
1:A:129:ARG:HG2	1:A:151:VAL:HB	1.87	0.57
1:B:190:THR:CG2	1:B:191:GLN:H	2.16	0.57
1:B:301:LEU:C	1:B:301:LEU:HD13	2.29	0.57
1:A:105:HIS:O	1:A:323:LYS:NZ	2.38	0.57
1:A:279:LEU:HD22	1:A:312:ARG:HD3	1.86	0.56
1:B:54:SER:HB2	1:B:56:THR:HG23	1.85	0.56
1:B:91:PRO:CB	1:B:143:THR:HG22	2.35	0.56
1:B:256:GLU:O	1:B:259:ASN:N	2.38	0.56
1:B:355:ILE:HB	1:B:372:LEU:HD21	1.86	0.56
1:B:151:VAL:O	1:B:151:VAL:HG22	2.03	0.56
1:B:129:ARG:CB	1:B:139:HIS:NE2	2.69	0.56
1:A:116:LEU:HD22	1:A:116:LEU:O	2.05	0.56
1:B:243:PRO:HA	1:B:250:ILE:CG1	2.35	0.56
1:A:188:LYS:O	1:A:189:VAL:C	2.48	0.56
1:A:181:GLY:O	1:A:185:LYS:HB2	2.05	0.56
1:A:230:ALA:C	1:A:232:ALA:N	2.64	0.56
1:B:90:ILE:CD1	1:B:160:ILE:HD13	2.36	0.56
1:B:268:VAL:HG23	3:B:377:NAD:H51N	1.86	0.56
1:B:26:VAL:HG22	1:B:132:CYS:HB2	1.87	0.56
1:B:243:PRO:CB	1:B:250:ILE:HG13	2.36	0.56
1:A:157:VAL:HG13	1:A:157:VAL:O	2.07	0.55
1:A:173:GLY:O	1:A:174:CYS:HB2	2.04	0.55
1:B:179:GLY:HA2	1:B:207:VAL:HG22	1.88	0.55
1:A:279:LEU:CD2	1:A:312:ARG:HD3	2.36	0.55
1:B:129:ARG:CB	1:B:139:HIS:CE1	2.85	0.55
1:A:252:GLU:O	1:A:256:GLU:N	2.39	0.55
1:B:282:CYS:O	1:B:312:ARG:NH1	2.39	0.55
1:A:35:GLU:HG2	1:A:123:MET:CE	2.36	0.55
1:B:41:VAL:O	1:B:374:PHE:HB2	2.06	0.55
1:A:140:PHE:HD1	1:A:141:LEU:N	2.05	0.55
1:A:293:GLY:O	1:B:309:LEU:HD11	2.07	0.55
1:B:218:ARG:NH2	1:B:220:ILE:HD11	2.20	0.55
1:A:295:PRO:CG	1:B:305:PRO:HG2	2.37	0.55
1:B:83:VAL:HG12	1:B:159:LYS:HB2	1.89	0.55
1:B:196:ALA:HB2	1:B:262:VAL:HG21	1.89	0.55
1:A:161:ASP:CB	1:A:164:SER:OG	2.55	0.54
1:B:141:LEU:C	1:B:143:THR:H	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:HD12	1:B:301:LEU:H	1.73	0.54
1:B:171:LEU:HD11	1:B:369:ARG:CG	2.37	0.54
1:B:283:GLN:HG2	1:B:286:TYR:CE2	2.41	0.54
1:A:363:ARG:CG	1:A:364:SER:N	2.70	0.54
1:B:89:VAL:HG13	1:B:158:ALA:H	1.73	0.54
1:B:129:ARG:CG	1:B:151:VAL:CG1	2.86	0.54
1:B:205:LEU:HD11	1:B:231:LYS:HB2	1.90	0.54
1:B:301:LEU:O	1:B:301:LEU:HD12	2.05	0.54
1:B:343:ASP:C	1:B:345:LEU:N	2.66	0.54
1:A:181:GLY:HA3	1:A:322:PHE:CE2	2.43	0.54
1:A:243:PRO:CB	1:A:250:ILE:HG13	2.28	0.54
1:B:45:ILE:CG1	1:B:370:THR:HG23	2.30	0.54
1:B:59:THR:CG2	1:B:60:PRO:N	2.70	0.54
1:A:272:LEU:HD12	1:B:305:PRO:CG	2.37	0.54
1:A:177:SER:HB3	1:A:331:LEU:HD13	1.90	0.53
1:B:231:LYS:C	1:B:235:VAL:HG22	2.32	0.53
1:A:17:GLU:O	1:A:18:LYS:CB	2.56	0.53
1:B:265:SER:OG	1:B:278:ALA:HB1	2.08	0.53
1:B:262:VAL:HG12	1:B:263:ASP:N	2.24	0.53
1:A:129:ARG:HG2	1:A:151:VAL:CB	2.39	0.53
1:A:179:GLY:HA2	1:A:207:VAL:CG2	2.31	0.53
1:A:359:PHE:O	1:A:363:ARG:HG2	2.09	0.53
1:B:88:LYS:HD3	1:B:166:LEU:HD11	1.90	0.53
1:A:168:LYS:O	1:A:170:CYS:N	2.39	0.53
1:B:204:GLY:N	1:B:268:VAL:HG21	2.24	0.53
1:A:371:ILE:HG22	1:A:371:ILE:O	2.07	0.53
1:B:195:CYS:HB3	1:B:266:PHE:CE1	2.38	0.52
1:B:345:LEU:O	1:B:368:ILE:CG2	2.57	0.52
1:A:285:ALA:CB	1:B:102:VAL:HG13	2.39	0.52
1:A:123:MET:HB2	1:A:127:THR:O	2.09	0.52
1:A:160:ILE:CG1	1:A:161:ASP:H	2.22	0.52
1:B:59:THR:HG22	1:B:60:PRO:N	2.23	0.52
1:B:154:GLU:O	1:B:154:GLU:HG2	2.09	0.52
1:B:258:SER:O	1:B:259:ASN:C	2.53	0.52
1:A:140:PHE:CE1	1:A:141:LEU:CG	2.88	0.52
1:A:10:LYS:HA	1:A:24:GLU:O	2.10	0.52
1:A:96:GLN:O	1:A:155:ILE:HB	2.09	0.52
1:B:48:SER:HB3	4:B:378:DMS:H12	1.92	0.52
1:B:73:VAL:HG23	1:B:87:ASP:O	2.09	0.52
1:A:68:GLU:HG3	1:A:174:CYS:CB	2.38	0.52
1:A:158:ALA:HB3	1:A:328:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASP:CA	1:A:339:LYS:HG2	2.40	0.52
1:A:176:PHE:CE2	1:A:209:MET:HE2	2.44	0.52
1:B:169:VAL:CG1	1:B:332:VAL:CG2	2.86	0.52
1:A:23:ILE:CD1	1:A:353:GLU:CA	2.69	0.51
1:A:295:PRO:CB	1:A:296:PRO:HD2	2.40	0.51
1:A:114:ASN:HD22	1:A:116:LEU:H	1.57	0.51
1:A:363:ARG:C	1:A:365:GLY:H	2.16	0.51
1:B:343:ASP:O	1:B:345:LEU:N	2.44	0.51
1:B:61:LEU:CD1	1:B:63:VAL:HG12	2.41	0.51
1:A:179:GLY:O	1:A:207:VAL:CG2	2.58	0.51
1:A:290:VAL:HG22	1:A:315:LYS:HB2	1.92	0.51
1:B:90:ILE:CG1	1:B:160:ILE:CD1	2.82	0.51
1:B:113:LYS:HE2	1:B:124:GLN:NE2	2.25	0.51
1:A:190:THR:CG2	1:A:264:PHE:HZ	2.22	0.51
1:A:346:ILE:HG22	1:A:346:ILE:O	2.09	0.51
1:B:16:GLU:HB3	1:B:19:LYS:CG	2.38	0.51
1:B:222:VAL:HG21	1:B:254:LEU:HD11	1.92	0.51
1:B:59:THR:HA	1:B:119:PRO:HB2	1.92	0.51
1:B:203:VAL:CG2	1:B:268:VAL:CG2	2.89	0.51
1:A:328:VAL:N	1:A:329:PRO:CD	2.74	0.51
1:A:346:ILE:HA	1:A:369:ARG:O	2.11	0.51
1:B:9:CYS:HB2	1:B:148:GLN:OE1	2.10	0.51
1:B:236:GLY:O	1:B:237:ALA:O	2.28	0.51
1:A:59:THR:OG1	1:A:60:PRO:HD2	2.11	0.50
1:A:129:ARG:HD2	1:A:151:VAL:HG11	1.93	0.50
1:A:350:LEU:O	1:A:372:LEU:HA	2.11	0.50
1:A:200:LEU:CD1	1:A:223:ASP:HB2	2.41	0.50
1:A:335:PHE:HB2	1:A:340:PHE:CE2	2.46	0.50
1:B:122:THR:CG2	1:B:139:HIS:HB2	2.41	0.50
1:B:148:GLN:HA	1:B:374:PHE:CE2	2.46	0.50
1:B:282:CYS:HB2	1:B:287:GLY:HA3	1.93	0.50
1:A:60:PRO:HB2	1:A:138:HIS:NE2	2.27	0.50
1:B:190:THR:HG22	1:B:191:GLN:H	1.72	0.50
1:A:48:SER:OG	4:A:378:DMS:H23	2.11	0.50
1:A:355:ILE:HB	1:A:372:LEU:HD21	1.92	0.50
1:A:363:ARG:C	1:A:365:GLY:N	2.68	0.50
1:B:143:THR:HA	1:B:152:VAL:HG12	1.94	0.50
1:B:200:LEU:HD21	1:B:221:GLY:HA3	1.93	0.50
1:A:47:ARG:C	1:A:49:ASP:N	2.68	0.50
1:A:310:SER:HB3	1:B:110:PHE:CD2	2.47	0.50
1:B:63:VAL:HG22	1:B:64:ILE:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:PHE:O	1:B:323:LYS:O	2.30	0.50
1:A:129:ARG:HG2	1:A:151:VAL:HG21	1.94	0.50
1:A:184:VAL:O	1:A:184:VAL:CG1	2.60	0.50
1:A:225:ASN:ND2	1:A:227:ASP:HB2	2.27	0.50
1:A:308:LEU:HD22	1:A:312:ARG:O	2.12	0.50
1:B:322:PHE:O	1:B:323:LYS:C	2.55	0.50
1:A:74:GLU:O	1:A:85:PRO:HB3	2.12	0.49
1:B:122:THR:HG23	1:B:139:HIS:HB2	1.92	0.49
1:B:362:LEU:C	1:B:364:SER:H	2.20	0.49
1:A:268:VAL:HG13	1:A:292:VAL:CG1	2.42	0.49
1:A:303:MET:O	1:B:301:LEU:HD12	2.11	0.49
1:B:250:ILE:O	1:B:254:LEU:HB2	2.12	0.49
1:A:11:ALA:O	1:A:23:ILE:HA	2.12	0.49
1:A:123:MET:HE1	1:A:151:VAL:O	2.12	0.49
1:A:140:PHE:CD1	1:A:141:LEU:N	2.81	0.49
1:A:147:SER:O	1:A:374:PHE:CE2	2.65	0.49
1:A:166:LEU:HA	1:A:169:VAL:HG12	1.94	0.49
1:A:343:ASP:HB2	1:A:344:PRO:HD3	1.93	0.49
1:B:160:ILE:O	1:B:162:ALA:N	2.43	0.49
1:B:272:LEU:HD13	1:B:296:PRO:HD2	1.95	0.49
1:A:102:VAL:HG11	1:A:110:PHE:O	2.12	0.49
1:B:73:VAL:CG1	1:B:75:SER:O	2.61	0.49
1:B:154:GLU:HA	1:B:157:VAL:CG1	2.43	0.49
1:B:203:VAL:HG23	1:B:204:GLY:N	2.27	0.49
1:B:109:ASN:HD21	1:B:319:PHE:HB3	1.77	0.49
1:A:13:VAL:HG11	1:A:15:TRP:CE2	2.47	0.49
1:A:218:ARG:O	1:A:219:ILE:HG13	2.13	0.49
1:A:200:LEU:HD12	1:A:223:ASP:CB	2.42	0.49
1:B:13:VAL:HG12	1:B:14:LEU:N	2.28	0.49
1:B:154:GLU:HA	1:B:157:VAL:HG11	1.95	0.49
1:B:348:HIS:CD2	1:B:361:LEU:HD21	2.48	0.49
1:B:89:VAL:HG13	1:B:157:VAL:CG2	2.40	0.49
1:A:350:LEU:HD13	1:A:370:THR:CG2	2.43	0.48
1:B:115:ASP:OD1	1:B:120:ARG:N	2.39	0.48
1:B:176:PHE:CE1	1:B:340:PHE:CZ	3.01	0.48
1:A:93:PHE:CE1	1:A:174:CYS:SG	3.06	0.48
1:A:194:THR:HG21	1:A:258:SER:OG	2.14	0.48
1:A:339:LYS:CE	1:A:339:LYS:CA	2.88	0.48
1:B:322:PHE:C	1:B:323:LYS:O	2.54	0.48
1:A:195:CYS:SG	1:A:211:CYS:HB3	2.53	0.48
1:A:232:ALA:O	1:A:235:VAL:CG2	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HG13	1:A:37:ARG:CZ	2.44	0.48
1:A:352:PHE:CE2	1:A:374:PHE:CE2	3.02	0.48
1:B:31:PRO:HG3	1:B:37:ARG:HB2	1.96	0.48
1:B:121:GLY:C	1:B:122:THR:CG2	2.86	0.48
1:B:223:ASP:CG	3:B:377:NAD:H1B	2.39	0.48
1:A:309:LEU:HD12	1:B:291:ILE:HG22	1.95	0.48
1:B:93:PHE:HB2	1:B:141:LEU:HD23	1.96	0.48
1:A:31:PRO:HD3	1:A:37:ARG:HG2	1.95	0.48
1:A:352:PHE:C	1:A:355:ILE:HG22	2.38	0.48
1:A:353:GLU:CD	1:A:353:GLU:H	2.22	0.48
1:B:256:GLU:C	1:B:259:ASN:N	2.69	0.48
1:B:308:LEU:HD11	1:B:314:TRP:HB2	1.95	0.48
1:B:327:SER:N	1:B:329:PRO:HD2	2.29	0.48
1:A:23:ILE:HD12	1:A:353:GLU:HA	1.83	0.48
1:B:121:GLY:CA	1:B:138:HIS:CD2	2.85	0.48
1:A:35:GLU:OE1	1:A:129:ARG:NH1	2.47	0.48
1:A:169:VAL:O	1:A:169:VAL:CG1	2.61	0.48
1:B:19:LYS:N	1:B:19:LYS:CD	2.76	0.48
1:B:362:LEU:C	1:B:364:SER:N	2.72	0.48
1:A:310:SER:HA	1:B:318:ILE:HD12	1.95	0.47
1:A:327:SER:O	1:A:331:LEU:HB2	2.14	0.47
1:B:71:GLY:O	1:B:88:LYS:HA	2.13	0.47
1:A:5:LYS:CA	1:A:30:PRO:HG3	2.39	0.47
1:B:6:VAL:CG1	1:B:7:ILE:N	2.76	0.47
1:A:84:ARG:O	1:A:87:ASP:CG	2.57	0.47
1:A:316:GLY:HA3	1:B:308:LEU:O	2.14	0.47
1:B:6:VAL:HG12	1:B:7:ILE:N	2.29	0.47
1:B:200:LEU:HD12	1:B:223:ASP:HB2	1.96	0.47
1:A:200:LEU:HD21	1:A:221:GLY:HA3	1.96	0.47
1:B:133:ARG:HB3	1:B:134:GLY:H	1.55	0.47
1:A:168:LYS:C	1:A:170:CYS:H	2.19	0.47
1:B:210:GLY:O	1:B:214:ALA:N	2.30	0.47
1:B:243:PRO:HB3	1:B:250:ILE:CG1	2.45	0.47
1:B:169:VAL:CG1	1:B:169:VAL:O	2.62	0.47
1:B:15:TRP:HA	1:B:62:PRO:HB3	1.96	0.47
1:B:198:PHE:HB2	1:B:267:GLU:HA	1.97	0.47
1:B:295:PRO:CB	1:B:296:PRO:HD2	2.44	0.47
1:B:265:SER:O	1:B:289:SER:HA	2.15	0.47
1:B:304:ASN:C	1:B:306:MET:H	2.22	0.47
1:A:275:MET:SD	1:B:305:PRO:HB3	2.55	0.47
1:A:13:VAL:CG2	1:A:137:ILE:HG21	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:HD23	1:A:14:LEU:HA	1.86	0.46
1:B:284:GLU:HA	1:B:312:ARG:CZ	2.46	0.46
1:A:303:MET:CE	1:A:308:LEU:HG	2.46	0.46
1:B:331:LEU:O	1:B:334:ASP:HB2	2.15	0.46
1:A:143:THR:O	1:A:144:SER:C	2.57	0.46
1:A:168:LYS:HG2	1:A:335:PHE:CZ	2.46	0.46
1:B:39:LYS:CB	1:B:149:TYR:CE1	2.97	0.46
1:B:88:LYS:HG2	1:B:166:LEU:HD11	1.97	0.46
1:A:47:ARG:O	1:A:50:ASP:N	2.45	0.46
1:B:9:CYS:O	1:B:26:VAL:N	2.41	0.46
1:A:268:VAL:HG13	1:A:292:VAL:HG11	1.97	0.46
1:B:172:ILE:O	1:B:172:ILE:CG2	2.64	0.46
1:B:231:LYS:H	1:B:231:LYS:HG2	1.54	0.46
1:B:269:ILE:CD1	1:B:274:THR:HG21	2.36	0.46
1:B:304:ASN:O	1:B:306:MET:N	2.49	0.46
1:A:195:CYS:O	1:A:219:ILE:HA	2.16	0.46
1:A:205:LEU:CA	1:A:208:ILE:HG23	2.46	0.46
1:A:285:ALA:CB	1:B:102:VAL:CG1	2.94	0.46
1:B:348:HIS:HE1	1:B:366:GLU:O	1.99	0.46
1:A:305:PRO:HG2	1:B:272:LEU:HD11	1.98	0.45
1:B:63:VAL:CG2	1:B:64:ILE:N	2.79	0.45
1:B:69:ALA:HA	1:B:170:CYS:HB2	1.98	0.45
1:B:201:GLY:O	1:B:205:LEU:HB2	2.17	0.45
1:B:256:GLU:HA	1:B:259:ASN:HA	1.97	0.45
1:B:195:CYS:CB	1:B:266:PHE:HE1	2.26	0.45
1:B:230:ALA:O	1:B:231:LYS:C	2.59	0.45
1:A:152:VAL:HG23	1:A:153:ASP:O	2.16	0.45
1:A:232:ALA:HA	1:A:235:VAL:HG22	1.96	0.45
1:A:249:PRO:HG2	1:A:252:GLU:OE1	2.16	0.45
1:A:303:MET:HG2	1:A:304:ASN:N	2.22	0.45
1:A:332:VAL:C	1:A:334:ASP:H	2.25	0.45
1:A:295:PRO:CB	1:A:296:PRO:CD	2.95	0.45
1:B:13:VAL:CG1	1:B:14:LEU:N	2.79	0.45
1:B:203:VAL:C	1:B:205:LEU:H	2.23	0.45
1:B:238:THR:OG1	1:B:239:GLU:N	2.49	0.45
1:A:118:MET:HA	1:A:119:PRO:HD2	1.71	0.45
1:A:335:PHE:CE2	1:A:342:LEU:HD22	2.51	0.45
1:A:295:PRO:HG3	1:B:305:PRO:HG2	1.98	0.45
1:B:231:LYS:HE2	1:B:344:PRO:O	2.17	0.45
1:A:305:PRO:HB2	1:B:275:MET:CE	2.46	0.45
1:B:198:PHE:CD1	1:B:274:THR:HG23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:O	1:A:219:ILE:CG1	2.65	0.45
1:B:361:LEU:HB3	1:B:367:SER:HB2	1.98	0.45
1:B:23:ILE:HD12	1:B:353:GLU:HA	1.88	0.45
1:B:90:ILE:CD1	1:B:160:ILE:CD1	2.95	0.45
1:B:355:ILE:C	1:B:357:GLU:N	2.74	0.45
1:B:94:THR:HG21	1:B:319:PHE:HB2	1.99	0.44
1:B:169:VAL:HG11	1:B:332:VAL:HG22	1.96	0.44
1:B:174:CYS:HB3	1:B:175:GLY:H	1.53	0.44
1:B:252:GLU:O	1:B:253:VAL:C	2.60	0.44
1:B:248:LYS:HD3	1:B:253:VAL:HG23	1.99	0.44
1:A:267:GLU:HG2	1:A:274:THR:HG22	1.99	0.44
1:B:225:ASN:C	1:B:227:ASP:N	2.75	0.44
1:B:323:LYS:O	1:B:327:SER:OG	2.36	0.44
1:A:43:THR:HG23	1:A:69:ALA:HB2	1.98	0.44
1:A:62:PRO:O	1:A:138:HIS:CB	2.50	0.44
1:B:61:LEU:HA	1:B:62:PRO:C	2.43	0.44
1:B:209:MET:HE2	1:B:235:VAL:HB	1.99	0.44
1:B:347:THR:CG2	1:B:368:ILE:HB	2.48	0.44
1:A:64:ILE:O	1:A:65:ALA:O	2.35	0.44
1:A:189:VAL:HB	1:A:214:ALA:CB	2.47	0.44
1:A:250:ILE:O	1:A:254:LEU:HB2	2.18	0.44
1:A:347:THR:HG21	1:A:368:ILE:HG23	1.99	0.44
1:B:223:ASP:OD2	3:B:377:NAD:H1B	2.17	0.44
1:A:14:LEU:HD11	1:A:53:VAL:HA	1.99	0.44
1:B:52:VAL:HA	1:B:57:LEU:O	2.18	0.44
1:B:141:LEU:C	1:B:143:THR:N	2.75	0.44
1:B:200:LEU:O	1:B:228:LYS:HG2	2.17	0.44
1:A:147:SER:CB	1:A:149:TYR:O	2.59	0.43
1:A:262:VAL:CG2	1:A:264:PHE:O	2.65	0.43
1:B:248:LYS:HD3	1:B:253:VAL:CG2	2.47	0.43
1:B:343:ASP:N	1:B:344:PRO:CD	2.81	0.43
1:B:347:THR:HG23	1:B:368:ILE:HB	2.00	0.43
1:A:100:CYS:O	1:A:102:VAL:N	2.51	0.43
1:A:222:VAL:HG22	1:A:241:VAL:HG13	2.00	0.43
1:A:254:LEU:HD22	1:A:254:LEU:HA	1.74	0.43
1:A:304:ASN:HD21	1:A:306:MET:HB2	1.74	0.43
1:B:352:PHE:C	1:B:354:LYS:H	2.26	0.43
1:B:61:LEU:HD11	1:B:63:VAL:HG12	2.01	0.43
1:B:306:MET:HA	1:B:309:LEU:HB2	2.00	0.43
1:B:349:VAL:CG1	1:B:373:THR:HG22	2.46	0.43
1:A:334:ASP:HA	1:A:339:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLY:CA	1:B:268:VAL:HG21	2.48	0.43
1:B:294:VAL:HG23	3:B:377:NAD:H2N	2.00	0.43
1:B:361:LEU:CG	1:B:367:SER:HB2	2.49	0.43
1:A:23:ILE:HD13	1:A:353:GLU:HA	1.88	0.43
1:A:105:HIS:CE1	1:B:286:TYR:CD1	3.05	0.43
1:B:74:GLU:HB3	1:B:75:SER:H	1.18	0.43
1:A:35:GLU:CG	1:A:153:ASP:HA	2.48	0.43
1:A:128:SER:HA	1:A:139:HIS:NE2	2.33	0.43
1:B:131:THR:HA	1:B:136:PRO:HA	2.01	0.43
1:B:334:ASP:O	1:B:339:LYS:CB	2.67	0.43
1:A:338:LYS:HE3	1:A:338:LYS:HB3	1.49	0.43
1:A:81:THR:OG1	1:A:82:THR:N	2.52	0.42
1:A:351:PRO:O	1:A:352:PHE:C	2.61	0.42
1:A:355:ILE:HA	1:A:372:LEU:HD21	2.00	0.42
1:B:11:ALA:HB1	1:B:64:ILE:HD12	2.01	0.42
1:B:63:VAL:HG22	1:B:64:ILE:O	2.18	0.42
1:B:186:VAL:HG21	1:B:290:VAL:HG11	1.98	0.42
1:B:195:CYS:CA	1:B:264:PHE:O	2.67	0.42
1:B:284:GLU:O	1:B:310:SER:HB2	2.19	0.42
1:B:315:LYS:H	1:B:315:LYS:HG2	1.73	0.42
1:A:140:PHE:CD1	1:A:140:PHE:C	2.98	0.42
1:A:339:LYS:N	1:A:339:LYS:HD2	2.33	0.42
1:B:32:LYS:HB3	1:B:33:ALA:H	1.44	0.42
1:B:318:ILE:CG2	1:B:319:PHE:N	2.83	0.42
1:A:225:ASN:C	1:A:227:ASP:N	2.77	0.42
1:A:271:ARG:HB3	1:A:273:ASP:OD1	2.19	0.42
1:A:272:LEU:CD1	1:B:305:PRO:CG	2.97	0.42
1:B:6:VAL:CG1	1:B:27:GLU:HG3	2.50	0.42
1:A:319:PHE:HD1	1:A:319:PHE:HA	1.60	0.42
1:B:179:GLY:HA2	1:B:207:VAL:CG2	2.49	0.42
1:B:179:GLY:CA	1:B:207:VAL:HG22	2.48	0.42
1:A:10:LYS:HB2	1:A:10:LYS:HE2	1.54	0.42
1:B:349:VAL:HG12	1:B:373:THR:HG21	1.95	0.42
1:A:84:ARG:O	1:A:87:ASP:CB	2.67	0.42
1:A:93:PHE:HB2	1:A:141:LEU:HD13	2.01	0.42
1:B:361:LEU:HG	1:B:367:SER:HB2	2.01	0.42
1:A:232:ALA:C	1:A:237:ALA:HB3	2.44	0.42
1:A:220:ILE:HG23	1:A:239:GLU:HB3	2.02	0.42
1:B:39:LYS:HB2	1:B:149:TYR:CZ	2.54	0.42
1:B:97:CYS:SG	1:B:100:CYS:SG	3.18	0.42
1:A:23:ILE:C	1:A:24:GLU:HG2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:CYS:O	1:A:103:CYS:N	2.51	0.42
1:A:122:THR:HB	1:A:123:MET:H	1.65	0.42
1:A:187:ALA:HB2	1:A:266:PHE:CE2	2.55	0.42
1:A:213:ALA:C	1:A:215:GLY:H	2.27	0.42
1:A:334:ASP:CB	1:A:339:LYS:HG2	2.50	0.42
1:B:54:SER:CB	1:B:56:THR:HG23	2.48	0.42
1:B:116:LEU:HD12	1:B:116:LEU:O	2.19	0.42
1:A:43:THR:OG1	1:A:374:PHE:CE1	2.73	0.41
1:A:100:CYS:HB2	1:A:112:LEU:HD22	2.01	0.41
1:A:141:LEU:HD11	4:A:378:DMS:H11	2.02	0.41
1:A:241:VAL:HG23	1:A:246:TYR:HE1	1.84	0.41
1:A:355:ILE:HB	1:A:372:LEU:HD23	2.00	0.41
1:A:90:ILE:HD13	1:A:90:ILE:HG21	1.81	0.41
1:A:172:ILE:C	1:A:174:CYS:H	2.27	0.41
1:B:171:LEU:CD1	1:B:371:ILE:HD11	2.50	0.41
1:B:231:LYS:HE2	1:B:231:LYS:HB3	1.73	0.41
1:A:275:MET:SD	1:B:305:PRO:CB	3.08	0.41
1:A:286:TYR:CD1	1:B:105:HIS:CE1	3.08	0.41
1:B:43:THR:HG23	1:B:69:ALA:HB2	2.02	0.41
1:A:347:THR:CG2	1:A:368:ILE:HG23	2.51	0.41
1:B:49:ASP:OD2	1:B:66:GLY:HA2	2.21	0.41
1:B:169:VAL:O	1:B:169:VAL:HG12	2.19	0.41
1:B:213:ALA:C	1:B:215:GLY:H	2.24	0.41
1:B:230:ALA:C	1:B:232:ALA:N	2.74	0.41
1:B:152:VAL:HB	1:B:153:ASP:H	1.72	0.41
1:B:288:VAL:CG1	1:B:315:LYS:HD3	2.50	0.41
1:B:352:PHE:O	1:B:353:GLU:CB	2.55	0.41
1:A:304:ASN:C	1:A:306:MET:H	2.29	0.41
1:B:72:ILE:CG2	1:B:87:ASP:N	2.83	0.41
1:B:328:VAL:HG22	1:B:329:PRO:CD	2.34	0.41
1:A:295:PRO:HB3	1:A:296:PRO:HD2	2.02	0.41
1:A:357:GLU:O	1:A:361:LEU:HG	2.20	0.41
1:B:129:ARG:CG	1:B:151:VAL:HG11	2.51	0.41
1:B:258:SER:OG	1:B:261:GLY:C	2.63	0.41
1:A:34:HIS:O	1:A:154:GLU:HB2	2.21	0.41
1:A:64:ILE:HB	1:A:144:SER:HB3	2.02	0.41
1:A:100:CYS:O	1:A:100:CYS:SG	2.79	0.41
1:A:187:ALA:CB	1:A:266:PHE:CE2	3.04	0.41
1:A:203:VAL:HG12	1:A:268:VAL:HG11	2.02	0.41
1:A:275:MET:SD	1:A:291:ILE:HD12	2.61	0.41
1:B:115:ASP:OD1	1:B:120:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:HB3	4:A:378:DMS:H12	2.03	0.41
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.89	0.41
1:B:129:ARG:HG3	1:B:151:VAL:HG11	2.02	0.41
1:B:254:LEU:HD22	1:B:281:CYS:SG	2.61	0.41
1:B:256:GLU:HA	1:B:259:ASN:CA	2.51	0.41
1:B:342:LEU:HD12	1:B:342:LEU:HA	1.88	0.41
1:A:307:LEU:HD12	1:A:307:LEU:HA	1.85	0.41
1:B:10:LYS:HB2	1:B:148:GLN:OE1	2.21	0.41
1:A:347:THR:HB	1:A:348:HIS:CE1	2.56	0.40
1:B:105:HIS:HD2	1:B:108:GLY:N	2.18	0.40
1:A:171:LEU:HD11	1:A:369:ARG:HG2	2.02	0.40
1:A:181:GLY:O	1:A:185:LYS:CB	2.70	0.40
1:A:208:ILE:HD11	1:A:237:ALA:HB2	1.97	0.40
1:B:88:LYS:HD3	1:B:166:LEU:CG	2.52	0.40
1:B:208:ILE:O	1:B:208:ILE:CG2	2.69	0.40
1:A:41:VAL:CG2	1:A:72:ILE:HD12	2.52	0.40
1:B:308:LEU:HA	1:B:308:LEU:HD12	1.79	0.40
1:A:94:THR:O	1:A:324:SER:OG	2.39	0.40
1:A:161:ASP:HB3	1:A:162:ALA:H	1.64	0.40
1:B:205:LEU:HD13	1:B:235:VAL:HG21	2.02	0.40
1:B:225:ASN:O	1:B:226:LYS:C	2.64	0.40

All (63) 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:A:248:LYS:NZ	1:B:245:ASP:OD1[1_655]	0.31	1.89
1:B:16:GLU:OE2	1:B:81:THR:CG2[1_545]	0.68	1.52
1:A:245:ASP:O	1:B:248:LYS:CB[1_655]	0.71	1.49
1:A:247:LYS:N	1:B:247:LYS:N[1_655]	0.72	1.48
1:A:248:LYS:CD	1:B:245:ASP:CB[1_655]	0.75	1.45
1:A:245:ASP:C	1:B:248:LYS:CG[1_655]	0.81	1.39
1:A:245:ASP:O	1:B:248:LYS:CG[1_655]	0.95	1.25
1:A:248:LYS:NZ	1:B:245:ASP:CG[1_655]	1.05	1.15
1:A:248:LYS:CG	1:B:245:ASP:C[1_655]	1.06	1.14
1:B:19:LYS:CE	1:B:81:THR:O[1_545]	1.07	1.13
1:B:19:LYS:NZ	1:B:81:THR:O[1_545]	1.14	1.06
1:A:248:LYS:CE	1:B:245:ASP:CG[1_655]	1.18	1.02
1:A:248:LYS:CG	1:B:245:ASP:O[1_655]	1.18	1.02
1:A:246:TYR:O	1:B:247:LYS:CG[1_655]	1.19	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LYS:CB	1:B:246:TYR:O[1_655]	1.26	0.94
1:B:16:GLU:CD	1:B:81:THR:CG2[1_545]	1.33	0.87
1:A:247:LYS:CA	1:B:247:LYS:N[1_655]	1.41	0.79
1:A:247:LYS:CB	1:B:246:TYR:C[1_655]	1.45	0.75
1:A:245:ASP:CB	1:B:248:LYS:CE[1_655]	1.47	0.73
1:A:218:ARG:NH2	1:B:239:GLU:OE2[1_655]	1.48	0.72
1:A:248:LYS:CG	1:B:245:ASP:CA[1_655]	1.50	0.70
1:A:17:GLU:OE2	1:A:337:ALA:O[1_545]	1.52	0.68
1:A:248:LYS:CE	1:B:245:ASP:OD1[1_655]	1.52	0.68
1:A:248:LYS:CE	1:B:245:ASP:CB[1_655]	1.55	0.65
1:A:248:LYS:CB	1:B:245:ASP:O[1_655]	1.56	0.64
1:B:16:GLU:OE2	1:B:81:THR:CB[1_545]	1.58	0.62
1:A:246:TYR:N	1:B:248:LYS:CG[1_655]	1.61	0.59
1:A:247:LYS:N	1:B:246:TYR:C[1_655]	1.63	0.57
1:A:17:GLU:OE2	1:A:337:ALA:C[1_545]	1.64	0.56
1:A:245:ASP:O	1:B:248:LYS:CA[1_655]	1.67	0.53
1:A:245:ASP:C	1:B:248:LYS:CB[1_655]	1.69	0.51
1:A:248:LYS:CG	1:B:245:ASP:CB[1_655]	1.69	0.51
1:A:246:TYR:O	1:B:247:LYS:CB[1_655]	1.71	0.49
1:A:233:LYS:NZ	1:B:259:ASN:OD1[1_655]	1.73	0.47
1:A:246:TYR:C	1:B:247:LYS:N[1_655]	1.75	0.45
1:A:248:LYS:CA	1:B:245:ASP:O[1_655]	1.78	0.42
1:A:247:LYS:CA	1:B:246:TYR:C[1_655]	1.79	0.41
1:B:19:LYS:NZ	1:B:81:THR:C[1_545]	1.79	0.41
1:A:248:LYS:CB	1:B:245:ASP:C[1_655]	1.81	0.39
1:A:246:TYR:CD2	1:B:246:TYR:CD2[1_655]	1.87	0.33
1:A:248:LYS:CB	1:B:245:ASP:CA[1_655]	1.90	0.30
1:A:248:LYS:N	1:B:245:ASP:O[1_655]	1.90	0.30
1:A:248:LYS:NZ	1:B:245:ASP:OD2[1_655]	1.93	0.27
1:A:248:LYS:CD	1:B:245:ASP:CG[1_655]	1.94	0.26
1:A:247:LYS:CG	1:B:246:TYR:O[1_655]	1.95	0.25
1:B:16:GLU:OE1	1:B:81:THR:CG2[1_545]	1.95	0.25
1:A:17:GLU:O	1:A:338:LYS:CD[1_545]	1.96	0.24
1:A:25:GLU:OE1	1:B:72:ILE:CD1[1_544]	1.97	0.23
1:A:246:TYR:C	1:B:247:LYS:CG[1_655]	1.98	0.22
1:B:16:GLU:OE2	1:B:81:THR:OG1[1_545]	1.98	0.22
1:A:239:GLU:OE2	1:B:257:MET:CG[1_655]	2.00	0.20
1:A:247:LYS:N	1:B:247:LYS:CA[1_655]	2.00	0.20
1:A:248:LYS:CD	1:B:245:ASP:CA[1_655]	2.02	0.18
1:A:17:GLU:OE2	1:A:337:ALA:CA[1_545]	2.06	0.14
1:A:247:LYS:CA	1:B:247:LYS:CA[1_655]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:N	1:B:245:ASP:C[1_655]	2.09	0.11
1:A:247:LYS:CB	1:B:247:LYS:N[1_655]	2.11	0.09
1:A:247:LYS:CD	1:B:246:TYR:O[1_655]	2.11	0.09
1:A:245:ASP:C	1:B:248:LYS:CD[1_655]	2.12	0.08
1:A:245:ASP:CA	1:B:248:LYS:CG[1_655]	2.14	0.06
1:A:247:LYS:N	1:B:246:TYR:CA[1_655]	2.15	0.05
1:A:246:TYR:CE2	1:B:253:VAL:CG2[1_655]	2.16	0.04
1:A:245:ASP:O	1:B:248:LYS:N[1_655]	2.19	0.01

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	372/374 (100%)	281 (76%)	53 (14%)	38 (10%)	0	1
1	B	372/374 (100%)	282 (76%)	58 (16%)	32 (9%)	0	1
All	All	744/748 (100%)	563 (76%)	111 (15%)	70 (9%)	0	1

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	33	ALA
1	A	65	ALA
1	A	99	LYS
1	A	109	ASN
1	A	162	ALA
1	A	169	VAL
1	A	174	CYS
1	A	189	VAL
1	A	216	ALA
1	A	259	ASN
1	A	297	ASP

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Mol	Chain	Res	Type
1	A	298	SER
1	A	353	GLU
1	A	367	SER
1	B	6	VAL
1	B	112	LEU
1	B	128	SER
1	B	133	ARG
1	B	161	ASP
1	B	175	GLY
1	B	237	ALA
1	B	297	ASP
1	A	18	LYS
1	A	97	CYS
1	A	101	ARG
1	A	110	PHE
1	A	141	LEU
1	A	144	SER
1	A	161	ASP
1	A	175	GLY
1	A	293	GLY
1	A	352	PHE
1	B	18	LYS
1	B	34	HIS
1	B	174	CYS
1	B	202	GLY
1	B	259	ASN
1	B	323	LYS
1	B	353	GLU
1	A	2	THR
1	A	4	GLY
1	A	67	HIS
1	B	4	GLY
1	B	33	ALA
1	B	97	CYS
1	B	154	GLU
1	B	284	GLU
1	B	363	ARG
1	A	82	THR
1	A	134	GLY
1	A	153	ASP
1	A	188	LYS
1	A	284	GLU

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Mol	Chain	Res	Type
1	B	65	ALA
1	B	81	THR
1	B	123	MET
1	B	124	GLN
1	A	160	ILE
1	A	177	SER
1	B	95	PRO
1	B	262	VAL
1	B	365	GLY
1	A	142	GLY
1	A	219	ILE
1	B	305	PRO
1	B	356	ASN
1	A	311	GLY
1	B	152	VAL
1	B	236	GLY

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	308/308 (100%)	193 (63%)	115 (37%)	0	0
1	B	308/308 (100%)	176 (57%)	132 (43%)	0	0
All	All	616/616 (100%)	369 (60%)	247 (40%)	0	0

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	5	LYS
1	A	7	ILE
1	A	10	LYS
1	A	13	VAL
1	A	14	LEU
1	A	18	LYS

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Mol	Chain	Res	Type
1	A	22	SER
1	A	27	GLU
1	A	28	VAL
1	A	32	LYS
1	A	37	ARG
1	A	39	LYS
1	A	43	THR
1	A	48	SER
1	A	53	VAL
1	A	54	SER
1	A	56	THR
1	A	57	LEU
1	A	74	GLU
1	A	75	SER
1	A	76	ILE
1	A	78	GLU
1	A	82	THR
1	A	83	VAL
1	A	88	LYS
1	A	96	GLN
1	A	99	LYS
1	A	101	ARG
1	A	107	GLU
1	A	112	LEU
1	A	116	LEU
1	A	118	MET
1	A	120	ARG
1	A	124	GLN
1	A	128	SER
1	A	129	ARG
1	A	131	THR
1	A	135	LYS
1	A	139	HIS
1	A	147	SER
1	A	148	GLN
1	A	150	THR
1	A	152	VAL
1	A	153	ASP
1	A	160	ILE
1	A	164	SER
1	A	167	GLU
1	A	168	LYS

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Mol	Chain	Res	Type
1	A	169	VAL
1	A	171	LEU
1	A	178	THR
1	A	184	VAL
1	A	185	LYS
1	A	191	GLN
1	A	193	SER
1	A	208	ILE
1	A	212	LYS
1	A	220	ILE
1	A	222	VAL
1	A	226	LYS
1	A	231	LYS
1	A	235	VAL
1	A	238	THR
1	A	241	VAL
1	A	247	LYS
1	A	248	LYS
1	A	250	ILE
1	A	251	GLN
1	A	254	LEU
1	A	257	MET
1	A	258	SER
1	A	259	ASN
1	A	262	VAL
1	A	268	VAL
1	A	272	LEU
1	A	276	VAL
1	A	279	LEU
1	A	280	SER
1	A	283	GLN
1	A	291	ILE
1	A	297	ASP
1	A	299	GLN
1	A	302	SER
1	A	303	MET
1	A	304	ASN
1	A	306	MET
1	A	309	LEU
1	A	310	SER
1	A	313	THR
1	A	318	ILE

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Mol	Chain	Res	Type
1	A	319	PHE
1	A	323	LYS
1	A	324	SER
1	A	326	ASP
1	A	327	SER
1	A	328	VAL
1	A	330	LYS
1	A	331	LEU
1	A	336	MET
1	A	338	LYS
1	A	339	LYS
1	A	342	LEU
1	A	346	ILE
1	A	347	THR
1	A	355	ILE
1	A	356	ASN
1	A	360	ASP
1	A	364	SER
1	A	367	SER
1	A	368	ILE
1	A	369	ARG
1	A	371	ILE
1	A	372	LEU
1	A	373	THR
1	B	1	SER
1	B	7	ILE
1	B	10	LYS
1	B	14	LEU
1	B	18	LYS
1	B	19	LYS
1	B	23	ILE
1	B	26	VAL
1	B	27	GLU
1	B	34	HIS
1	B	36	VAL
1	B	37	ARG
1	B	39	LYS
1	B	40	MET
1	B	41	VAL
1	B	43	THR
1	B	45	ILE
1	B	46	CYS

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Mol	Chain	Res	Type
1	B	58	VAL
1	B	61	LEU
1	B	64	ILE
1	B	72	ILE
1	B	73	VAL
1	B	74	GLU
1	B	75	SER
1	B	76	ILE
1	B	80	VAL
1	B	82	THR
1	B	92	LEU
1	B	94	THR
1	B	96	GLN
1	B	97	CYS
1	B	99	LYS
1	B	100	CYS
1	B	102	VAL
1	B	103	CYS
1	B	104	LYS
1	B	107	GLU
1	B	109	ASN
1	B	110	PHE
1	B	112	LEU
1	B	113	LYS
1	B	114	ASN
1	B	115	ASP
1	B	116	LEU
1	B	117	SER
1	B	120	ARG
1	B	122	THR
1	B	124	GLN
1	B	125	ASP
1	B	129	ARG
1	B	133	ARG
1	B	135	LYS
1	B	141	LEU
1	B	143	THR
1	B	148	GLN
1	B	151	VAL
1	B	155	ILE
1	B	156	SER
1	B	157	VAL

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Mol	Chain	Res	Type
1	B	160	ILE
1	B	164	SER
1	B	167	GLU
1	B	168	LYS
1	B	169	VAL
1	B	171	LEU
1	B	172	ILE
1	B	174	CYS
1	B	185	LYS
1	B	186	VAL
1	B	188	LYS
1	B	189	VAL
1	B	191	GLN
1	B	195	CYS
1	B	197	VAL
1	B	205	LEU
1	B	206	SER
1	B	208	ILE
1	B	212	LYS
1	B	219	ILE
1	B	224	ILE
1	B	228	LYS
1	B	231	LYS
1	B	233	LYS
1	B	239	GLU
1	B	240	CYS
1	B	247	LYS
1	B	248	LYS
1	B	250	ILE
1	B	252	GLU
1	B	254	LEU
1	B	256	GLU
1	B	262	VAL
1	B	263	ASP
1	B	265	SER
1	B	268	VAL
1	B	272	LEU
1	B	275	MET
1	B	279	LEU
1	B	290	VAL
1	B	301	LEU
1	B	303	MET

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Mol	Chain	Res	Type
1	B	306	MET
1	B	308	LEU
1	B	309	LEU
1	B	310	SER
1	B	313	THR
1	B	315	LYS
1	B	318	ILE
1	B	319	PHE
1	B	323	LYS
1	B	324	SER
1	B	325	LYS
1	B	327	SER
1	B	328	VAL
1	B	330	LYS
1	B	332	VAL
1	B	336	MET
1	B	339	LYS
1	B	342	LEU
1	B	345	LEU
1	B	346	ILE
1	B	350	LEU
1	B	354	LYS
1	B	356	ASN
1	B	357	GLU
1	B	366	GLU
1	B	368	ILE
1	B	369	ARG
1	B	371	ILE
1	B	372	LEU
1	B	373	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	114	ASN
1	A	242	ASN
1	A	283	GLN
1	A	299	GLN
1	A	300	ASN
1	A	304	ASN
1	B	105	HIS

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Mol	Chain	Res	Type
1	B	109	ASN
1	B	124	GLN
1	B	138	HIS
1	B	225	ASN
1	B	283	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	$\# Z > 2$
4	DMS	A	378	2	3,3,3	0.57	0	3,3,3	0.16	0
3	NAD	A	377	-	46,48,48	1.45	6 (13%)	64,73,73	1.61	6 (9%)
3	NAD	B	377	-	46,48,48	1.94	6 (13%)	64,73,73	1.82	7 (10%)
4	DMS	B	378	2	3,3,3	0.61	0	3,3,3	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	377	-	-	9/30/62/62	0/5/5/5
3	NAD	B	377	-	-	10/30/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	377	NAD	C5B-C4B	-8.00	1.27	1.51
3	A	377	NAD	PN-O3	5.80	1.65	1.59
3	B	377	NAD	PN-O3	4.94	1.64	1.59
3	A	377	NAD	C3N-C7N	4.53	1.57	1.50
3	B	377	NAD	C1B-N9A	4.32	1.58	1.46
3	B	377	NAD	C3N-C7N	3.89	1.56	1.50
3	B	377	NAD	PA-O3	-3.37	1.55	1.59
3	B	377	NAD	C6N-N1N	2.49	1.41	1.35
3	A	377	NAD	PA-O3	-2.37	1.56	1.59
3	A	377	NAD	C6N-N1N	2.33	1.40	1.35
3	A	377	NAD	C2N-N1N	2.08	1.37	1.35
3	A	377	NAD	C2A-N3A	-2.01	1.30	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	377	NAD	C5N-C4N-C3N	-7.98	112.52	120.36
3	A	377	NAD	C5N-C4N-C3N	-7.46	113.03	120.36
3	B	377	NAD	C6N-C5N-C4N	5.88	127.92	119.45
3	A	377	NAD	C6N-C5N-C4N	5.75	127.74	119.45
3	B	377	NAD	O4B-C4B-C5B	5.19	125.96	109.33
3	B	377	NAD	C5N-C6N-N1N	-4.51	114.23	120.38
3	A	377	NAD	C5N-C6N-N1N	-4.07	114.83	120.38
3	B	377	NAD	C2N-C3N-C4N	3.78	122.66	118.26
3	A	377	NAD	C2N-C3N-C4N	3.76	122.63	118.26
3	B	377	NAD	O2A-PA-O3	2.65	114.44	107.27
3	A	377	NAD	O2A-PA-O3	2.34	113.59	107.27
3	B	377	NAD	C2B-C1B-N9A	-2.27	107.66	113.30
3	A	377	NAD	C4N-C3N-C7N	-2.19	115.09	121.06

There are no chirality outliers.

All (19) torsion outliers are listed below:

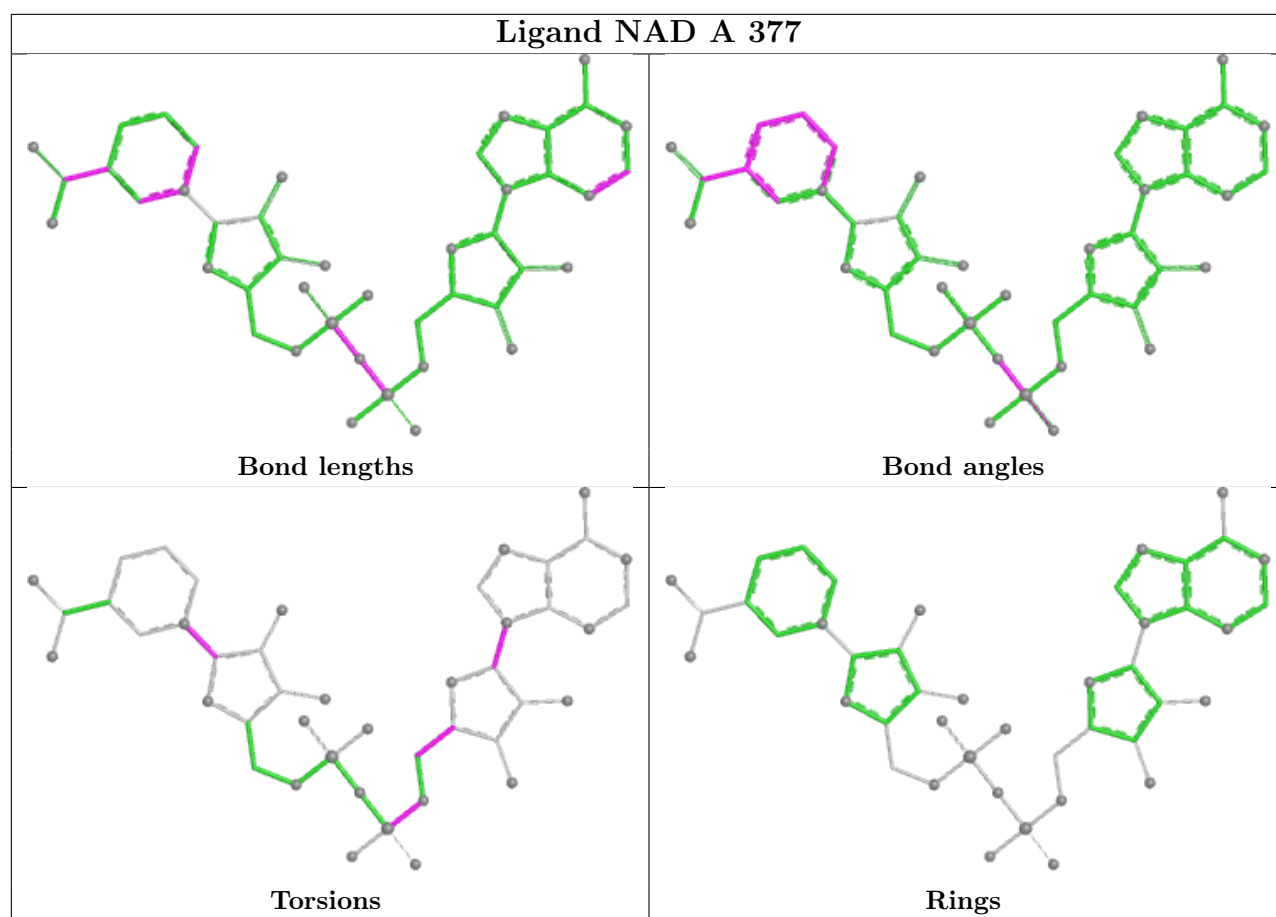
Mol	Chain	Res	Type	Atoms
3	A	377	NAD	C5B-O5B-PA-O1A
3	A	377	NAD	C5B-O5B-PA-O3
3	A	377	NAD	O4D-C1D-N1N-C2N
3	A	377	NAD	O4D-C1D-N1N-C6N
3	A	377	NAD	C2D-C1D-N1N-C2N
3	A	377	NAD	C2D-C1D-N1N-C6N
3	B	377	NAD	C5B-O5B-PA-O1A
3	B	377	NAD	C5B-O5B-PA-O3
3	B	377	NAD	O4D-C1D-N1N-C2N
3	B	377	NAD	O4D-C1D-N1N-C6N
3	B	377	NAD	C2D-C1D-N1N-C2N
3	B	377	NAD	C2D-C1D-N1N-C6N
3	B	377	NAD	O4B-C4B-C5B-O5B
3	B	377	NAD	C3B-C4B-C5B-O5B
3	A	377	NAD	C5B-O5B-PA-O2A
3	B	377	NAD	C5B-O5B-PA-O2A
3	A	377	NAD	O4B-C4B-C5B-O5B
3	A	377	NAD	C2B-C1B-N9A-C8A
3	B	377	NAD	C2B-C1B-N9A-C8A

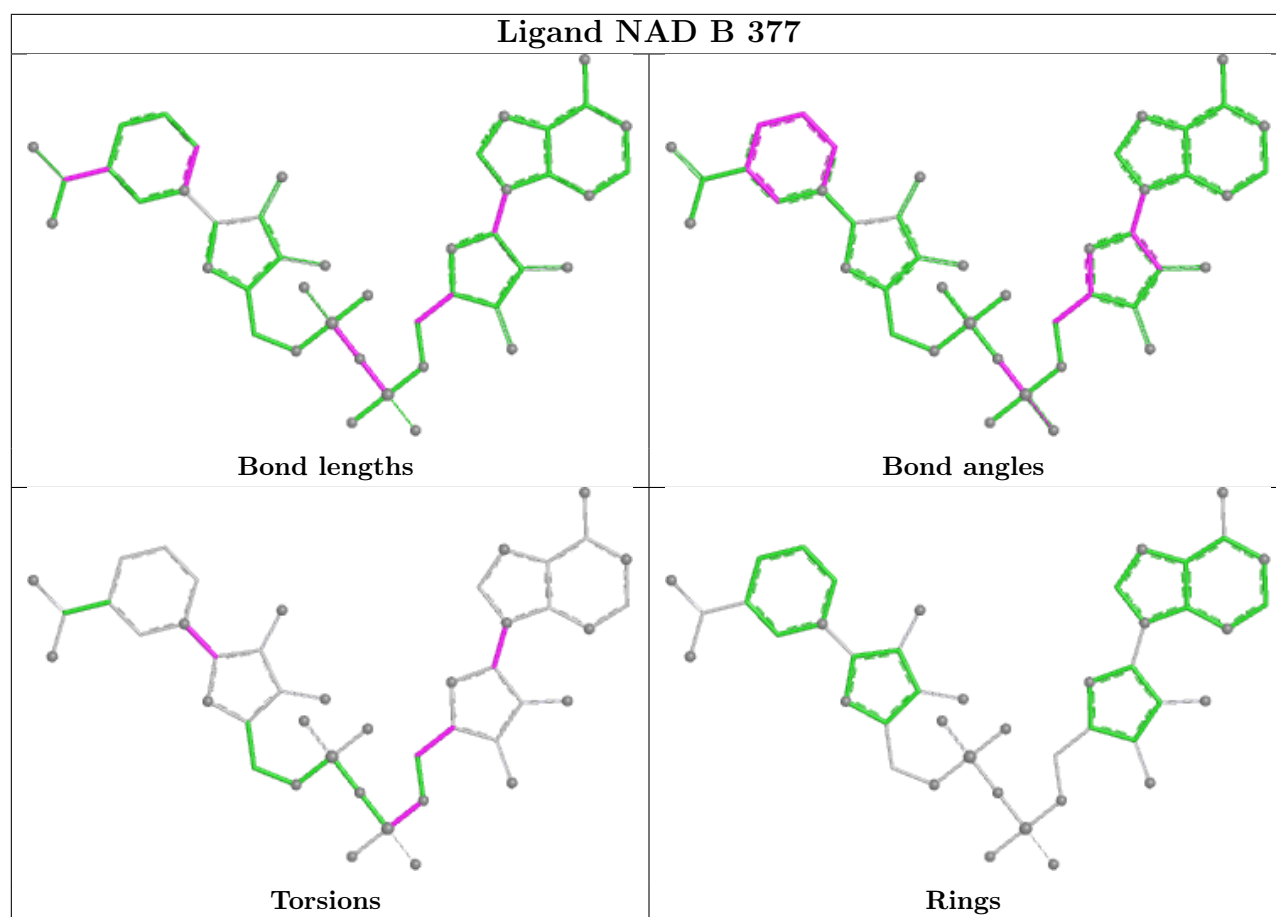
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	378	DMS	3	0
3	B	377	NAD	4	0
4	B	378	DMS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.