



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 04:09 AM UTC

PDB ID : 3H3F / pdb_00003h3f
Title : Rabbit muscle L-lactate dehydrogenase in complex with NADH and oxamate
Authors : Bujacz, A.; Bujacz, G.; Swiderek, K.; Paneth, P.
Deposited on : 2009-04-16
Resolution : 2.38 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

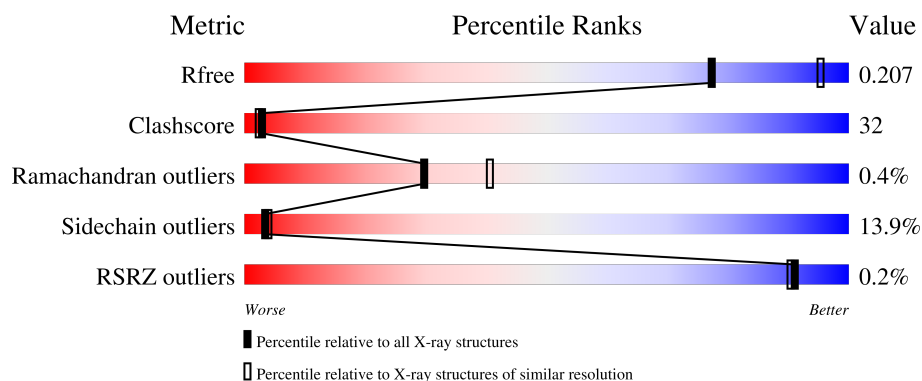
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	54% 35% 9% .
1	B	331	60% 33% 7% .
1	C	331	51% 37% 12%
1	D	331	54% 37% 8% .
1	E	331	% 46% 40% 12% .

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Mol	Chain	Length	Quality of chain
1	F	331	
1	G	331	
1	H	331	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXM	F	333	-	-	X	-
4	ACT	C	334	-	-	X	-
4	ACT	D	336	-	-	X	-

2 Entry composition

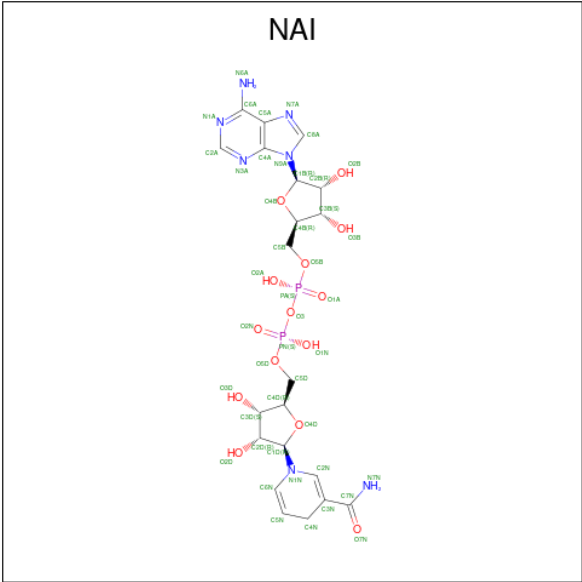
There are 5 unique types of molecules in this entry. The entry contains 22218 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lactate dehydrogenase A chain.

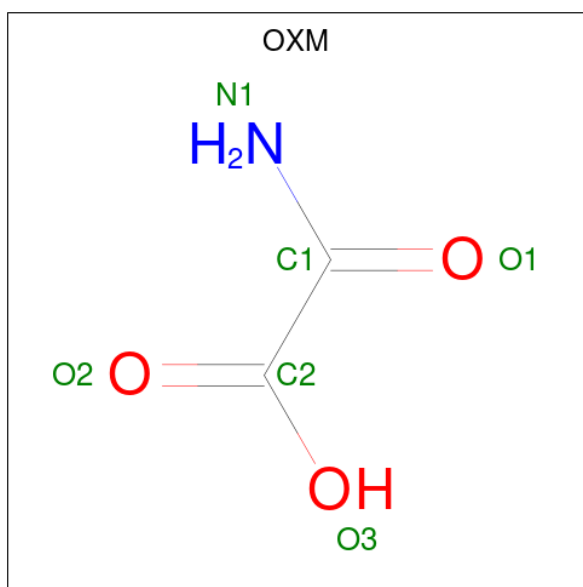
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	1	0
			2562	1635	442	471	14			
1	B	331	Total	C	N	O	S	0	2	0
			2568	1641	442	471	14			
1	C	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	D	331	Total	C	N	O	S	0	4	0
			2575	1644	442	475	14			
1	E	331	Total	C	N	O	S	0	1	0
			2564	1636	441	473	14			
1	F	331	Total	C	N	O	S	0	1	0
			2563	1636	441	471	15			
1	G	331	Total	C	N	O	S	0	3	0
			2571	1639	442	476	14			
1	H	331	Total	C	N	O	S	0	2	0
			2568	1640	441	473	14			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



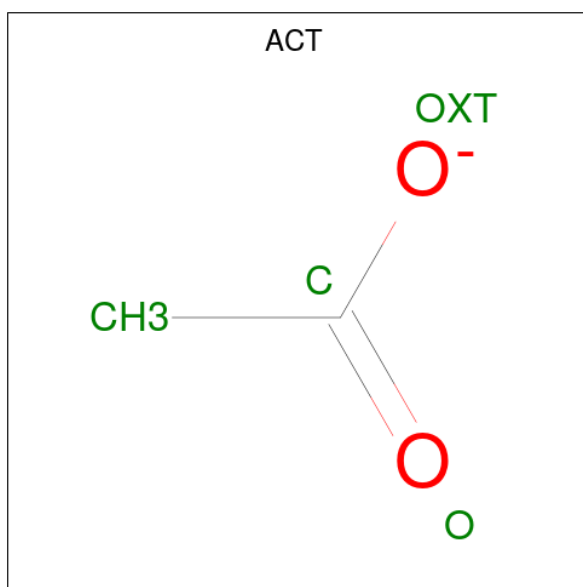
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G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

- Molecule 3 is OXAMIC ACID (CCD ID: OXM) (formula: C₂H₃NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	2	1	3		
3	B	1	Total	C	N	O	0	0
			6	2	1	3		
3	C	1	Total	C	N	O	0	0
			6	2	1	3		
3	D	1	Total	C	N	O	0	0
			6	2	1	3		
3	E	1	Total	C	N	O	0	0
			6	2	1	3		
3	F	1	Total	C	N	O	0	0
			6	2	1	3		
3	G	1	Total	C	N	O	0	0
			6	2	1	3		
3	H	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

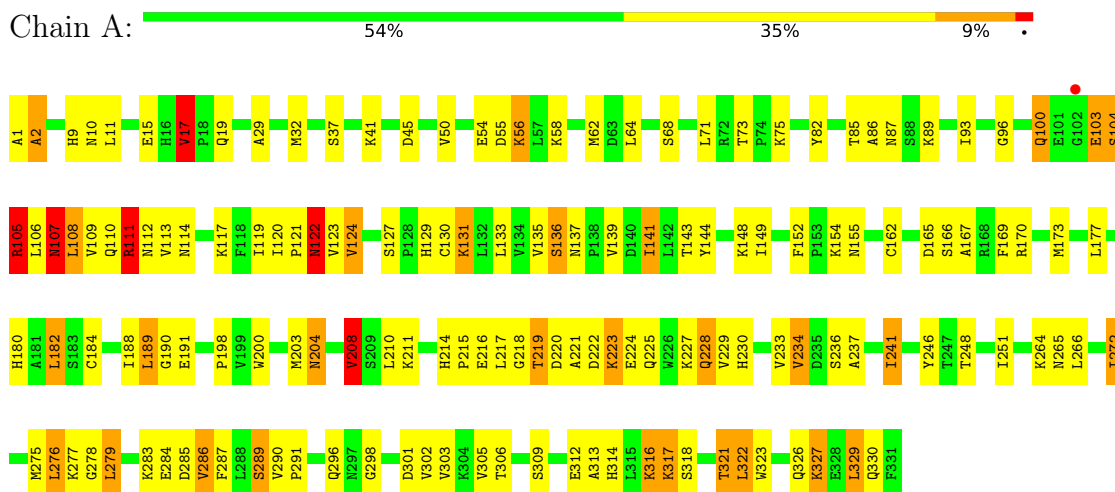
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	146	Total O 146 146	0	0
5	B	202	Total O 202 202	0	0
5	C	143	Total O 143 143	0	0
5	D	139	Total O 139 139	0	0
5	E	116	Total O 116 116	0	0
5	F	153	Total O 153 153	0	0
5	G	158	Total O 158 158	0	0
5	H	139	Total O 139 139	0	0

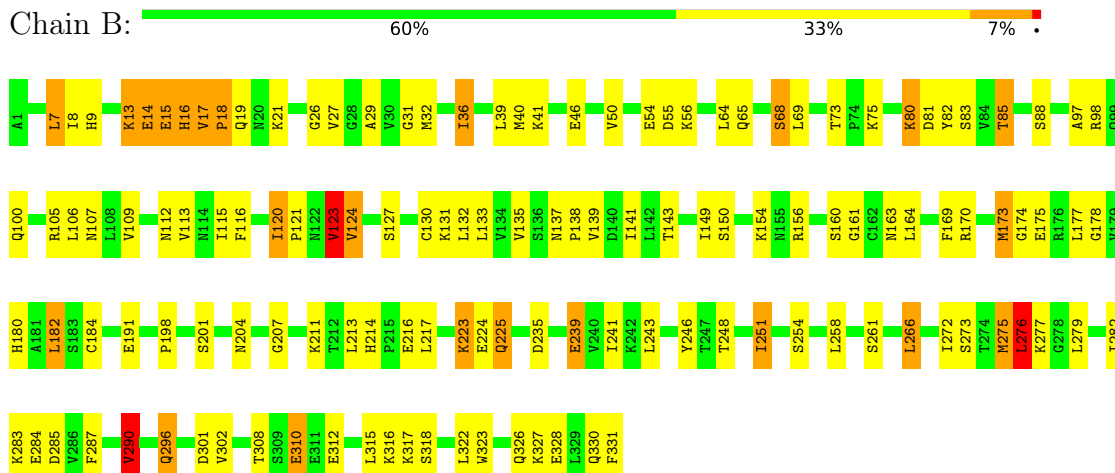
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: L-lactate dehydrogenase A chain

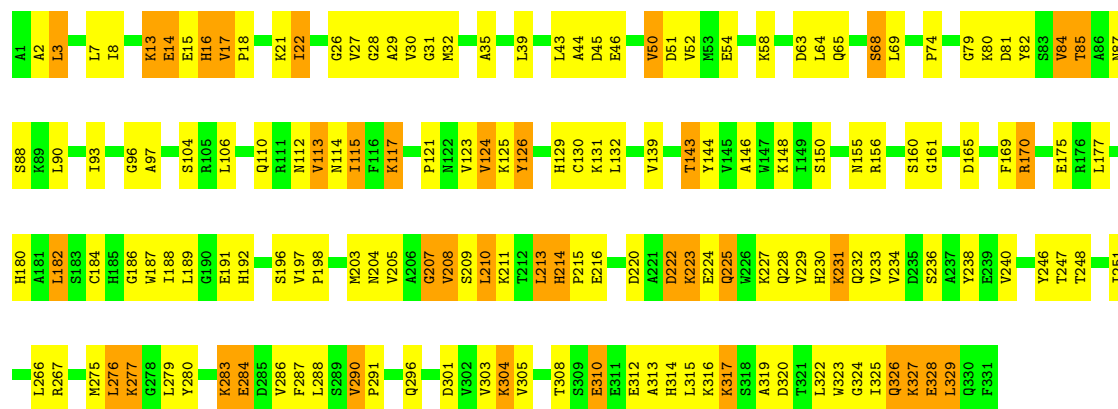


• Molecule 1: L-lactate dehydrogenase A chain



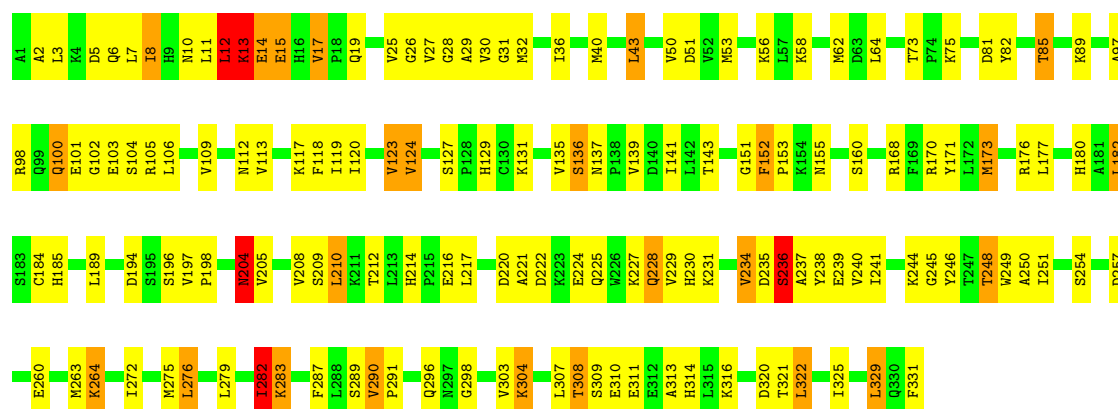
• Molecule 1: L-lactate dehydrogenase A chain





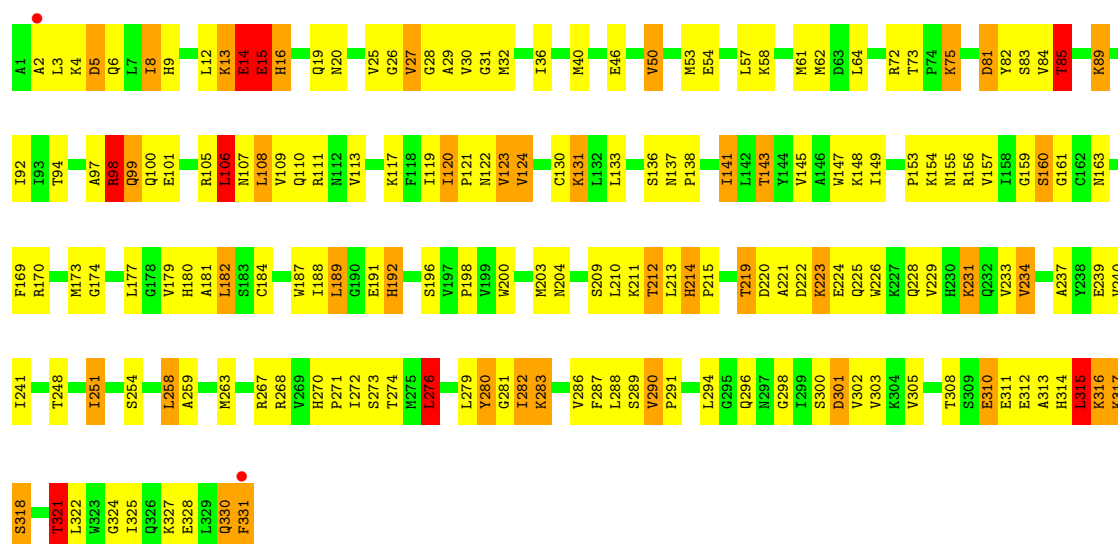
• Molecule 1: L-lactate dehydrogenase A chain

Chain D: 54% 37% 8% .



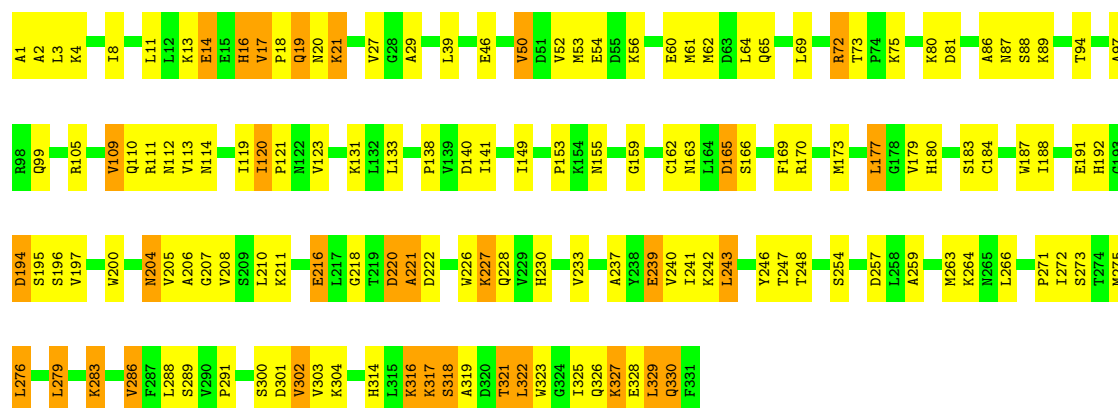
• Molecule 1: L-lactate dehydrogenase A chain

Chain E: 46% 40% 12% .



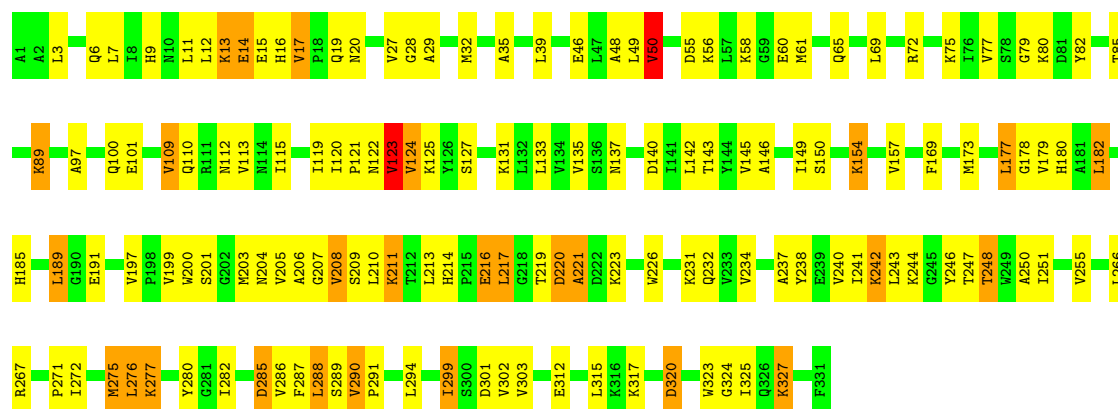
• Molecule 1: L-lactate dehydrogenase A chain

Chain F:  56% 34% 10%



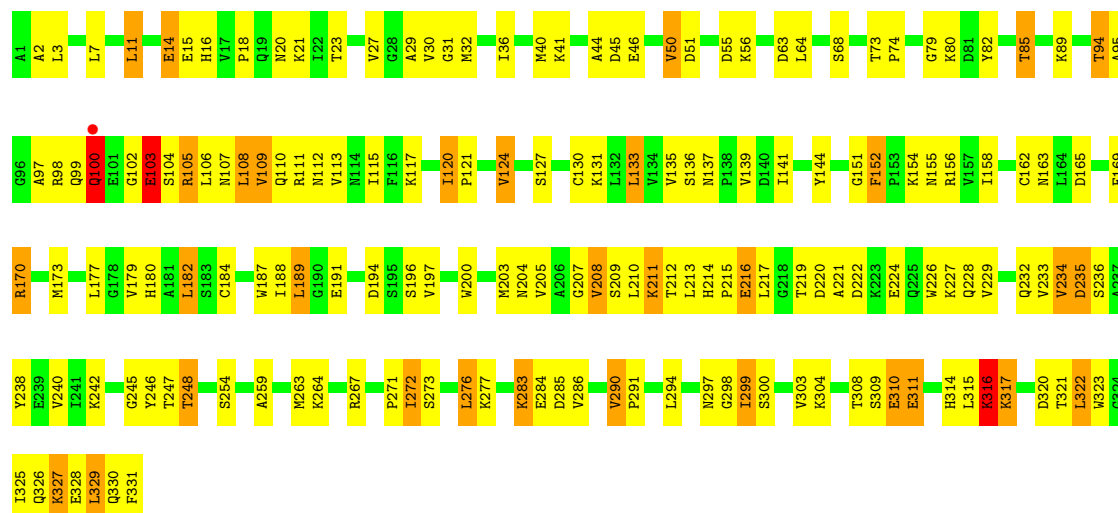
• Molecule 1: L-lactate dehydrogenase A chain

Chain G:  56% 35% 8%



• Molecule 1: L-lactate dehydrogenase A chain

Chain H:  48% 41% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.50Å 85.28Å 138.53Å 98.49° 91.67° 111.59°	Depositor
Resolution (Å)	60.00 – 2.38 60.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	89.7 (60.00-2.38) 89.6 (60.00-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.160 , 0.207 0.164 , 0.207	Depositor DCC
R_{free} test set	4887 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22218	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, ACT, OXM

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	1.15	4/2614 (0.2%)	1.31	21/3534 (0.6%)
1	B	1.23	6/2622 (0.2%)	1.38	30/3545 (0.8%)
1	C	1.14	3/2605 (0.1%)	1.34	20/3523 (0.6%)
1	D	1.12	0/2639	1.32	15/3568 (0.4%)
1	E	1.11	3/2613 (0.1%)	1.34	27/3534 (0.8%)
1	F	1.16	3/2613 (0.1%)	1.31	17/3533 (0.5%)
1	G	1.17	4/2632 (0.2%)	1.32	15/3559 (0.4%)
1	H	1.09	3/2622 (0.1%)	1.33	22/3546 (0.6%)
All	All	1.15	26/20960 (0.1%)	1.33	167/28342 (0.6%)

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	D	0	2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	ILE	CA-CB	11.92	1.60	1.54
1	F	120	ILE	CA-CB	-8.08	1.48	1.53
1	A	251	ILE	CA-CB	7.49	1.63	1.54
1	A	208	VAL	CA-CB	6.58	1.60	1.53
1	H	135	VAL	CA-CB	6.27	1.63	1.55
1	C	208	VAL	CA-CB	6.20	1.60	1.53
1	G	135	VAL	CA-CB	6.14	1.62	1.54
1	G	48	ALA	CA-C	5.96	1.60	1.52
1	B	241	ILE	CA-CB	5.95	1.61	1.54
1	C	290	VAL	CA-C	5.84	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	135	VAL	CA-C	5.84	1.58	1.52
1	C	143	THR	CA-CB	5.71	1.62	1.53
1	A	139	VAL	CA-CB	5.60	1.61	1.54
1	G	50	VAL	CA-CB	5.54	1.64	1.55
1	A	251	ILE	CA-C	5.50	1.59	1.52
1	B	120	ILE	C-O	-5.40	1.20	1.24
1	E	234	VAL	CA-CB	5.35	1.61	1.54
1	G	185	HIS	CA-C	-5.25	1.46	1.52
1	E	283	LYS	CA-C	5.22	1.59	1.52
1	F	197	VAL	N-CA	-5.20	1.42	1.46
1	E	92	ILE	CA-CB	-5.14	1.48	1.54
1	H	234	VAL	CA-CB	5.02	1.60	1.54
1	H	73	THR	C-O	-5.02	1.21	1.25
1	B	113	VAL	CA-CB	-5.01	1.48	1.54
1	B	201	SER	CA-C	5.01	1.59	1.52
1	F	50	VAL	CA-CB	5.01	1.61	1.54

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	109	VAL	N-CA-C	-10.68	101.02	110.74
1	D	13	LYS	N-CA-C	10.10	125.03	108.26
1	A	152	PHE	CA-C-N	-9.01	111.11	120.03
1	A	152	PHE	C-N-CA	-9.01	111.11	120.03
1	E	120	ILE	CA-C-N	8.90	128.55	118.85
1	E	120	ILE	C-N-CA	8.90	128.55	118.85
1	E	16	HIS	N-CA-C	8.76	124.45	107.98
1	H	135	VAL	N-CA-C	-7.92	106.18	113.71
1	G	280	TYR	N-CA-C	7.79	122.12	112.47
1	F	120	ILE	N-CA-CB	7.69	115.35	110.50
1	E	106	LEU	N-CA-C	-7.62	103.99	113.28
1	E	212	THR	N-CA-C	-7.39	103.25	111.82
1	H	73	THR	CA-C-N	-7.34	112.01	120.89
1	H	73	THR	C-N-CA	-7.34	112.01	120.89
1	F	73	THR	CA-C-N	-7.33	112.63	120.47
1	F	73	THR	C-N-CA	-7.33	112.63	120.47
1	B	127	SER	CA-C-N	7.25	128.91	119.84
1	B	127	SER	C-N-CA	7.25	128.91	119.84
1	E	196	SER	CA-C-N	-7.25	117.02	123.33
1	E	196	SER	C-N-CA	-7.25	117.02	123.33
1	H	197	VAL	N-CA-C	7.22	115.33	107.60
1	H	103	GLU	N-CA-C	7.19	120.81	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	VAL	N-CA-C	7.09	117.88	110.72
1	F	289	SER	N-CA-C	7.04	120.02	109.25
1	A	266	LEU	N-CA-C	6.93	118.84	111.28
1	E	123	VAL	N-CA-CB	6.89	119.40	110.57
1	B	18	PRO	N-CA-C	-6.79	99.71	111.32
1	D	263	MET	N-CA-C	6.79	118.68	111.28
1	H	80	LYS	N-CA-C	-6.78	104.82	113.23
1	C	214	HIS	CA-C-N	6.76	126.45	119.56
1	C	214	HIS	C-N-CA	6.76	126.45	119.56
1	B	100	GLN	N-CA-C	-6.74	101.45	110.55
1	G	127	SER	CA-C-N	-6.74	113.22	119.82
1	G	127	SER	C-N-CA	-6.74	113.22	119.82
1	E	280	TYR	N-CA-C	-6.73	104.20	113.56
1	A	107	ASN	N-CA-C	-6.73	103.87	111.14
1	F	275	MET	CA-C-N	-6.68	113.22	123.17
1	F	275	MET	C-N-CA	-6.68	113.22	123.17
1	G	16	HIS	N-CA-C	6.58	119.57	107.99
1	F	204	ASN	N-CA-C	6.52	118.12	108.60
1	H	290	VAL	CA-C-N	-6.48	112.25	120.23
1	H	290	VAL	C-N-CA	-6.48	112.25	120.23
1	A	275	MET	CA-C-N	-6.46	110.93	123.13
1	A	275	MET	C-N-CA	-6.46	110.93	123.13
1	D	12	LEU	CA-C-N	-6.40	112.91	122.39
1	D	12	LEU	C-N-CA	-6.40	112.91	122.39
1	H	152	PHE	N-CA-C	-6.39	101.79	110.36
1	E	89	LYS	N-CA-C	-6.38	104.55	112.90
1	B	272	ILE	CA-C-N	-6.38	113.15	122.65
1	B	272	ILE	C-N-CA	-6.38	113.15	122.65
1	D	290	VAL	CA-C-N	-6.34	113.24	119.90
1	D	290	VAL	C-N-CA	-6.34	113.24	119.90
1	B	116	PHE	N-CA-C	6.26	118.10	111.28
1	F	120	ILE	CA-C-N	-6.25	112.02	119.84
1	F	120	ILE	C-N-CA	-6.25	112.02	119.84
1	C	231	LYS	N-CA-C	-6.24	104.40	111.14
1	A	105	ARG	N-CA-C	-6.23	104.73	113.20
1	D	8	ILE	CB-CA-C	-6.19	101.61	110.83
1	E	276	LEU	N-CA-C	6.18	120.13	112.59
1	A	55	ASP	N-CA-C	-6.17	103.87	111.40
1	B	123	VAL	N-CA-CB	6.17	117.63	110.65
1	B	141	ILE	CB-CA-C	-6.11	104.15	111.97
1	H	300	SER	N-CA-C	6.10	119.92	112.23
1	A	122	ASN	CA-C-N	-6.09	112.11	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ASN	C-N-CA	-6.09	112.11	120.46
1	B	290	VAL	N-CA-CB	-6.09	102.69	111.21
1	B	273	SER	N-CA-C	6.08	119.73	109.76
1	A	139	VAL	N-CA-C	6.08	116.82	110.62
1	G	119	ILE	N-CA-C	6.07	116.19	110.30
1	C	16	HIS	N-CA-C	6.04	118.56	108.96
1	B	73	THR	CA-C-N	-6.03	113.76	120.45
1	B	73	THR	C-N-CA	-6.03	113.76	120.45
1	A	54	GLU	N-CA-C	6.00	117.90	111.36
1	D	100	GLN	N-CA-C	6.00	118.44	108.13
1	C	3	LEU	N-CA-C	-5.99	104.66	111.07
1	D	73	THR	N-CA-C	-5.95	95.53	108.74
1	E	258	LEU	N-CA-C	-5.93	104.72	111.07
1	G	137	ASN	N-CA-C	5.93	118.48	110.29
1	G	109	VAL	N-CA-C	5.92	116.39	110.23
1	E	214	HIS	CA-C-N	5.92	125.47	119.19
1	E	214	HIS	C-N-CA	5.92	125.47	119.19
1	D	204	ASN	N-CA-C	5.91	117.12	108.14
1	C	58	LYS	N-CA-C	5.86	118.61	111.82
1	B	17	VAL	CA-C-N	-5.85	113.67	119.99
1	B	17	VAL	C-N-CA	-5.85	113.67	119.99
1	E	98	ARG	N-CA-C	-5.85	100.14	109.96
1	E	84	VAL	N-CA-C	-5.84	105.41	113.00
1	B	36	ILE	N-CA-C	5.84	116.57	110.62
1	A	167	ALA	N-CA-C	-5.82	105.02	111.36
1	B	239	GLU	N-CA-C	-5.80	104.55	111.69
1	C	209	SER	N-CA-C	5.80	118.75	110.10
1	C	143	THR	N-CA-C	-5.78	104.89	111.14
1	D	236	SER	N-CA-C	5.78	117.58	111.28
1	F	302	VAL	CB-CA-C	-5.78	102.26	110.12
1	G	275	MET	CA-C-N	-5.77	114.57	123.17
1	G	275	MET	C-N-CA	-5.77	114.57	123.17
1	H	102	GLY	N-CA-C	-5.77	107.91	115.47
1	A	204	ASN	N-CA-C	5.75	117.81	109.07
1	F	109	VAL	CB-CA-C	-5.75	104.51	112.04
1	H	41	LYS	N-CA-C	-5.74	104.85	112.94
1	H	316	LYS	N-CA-C	-5.68	106.19	113.23
1	H	14	GLU	N-CA-C	5.67	118.42	108.56
1	E	15	GLU	N-CA-C	5.64	118.34	108.52
1	H	120	ILE	CA-C-N	5.58	125.26	119.56
1	H	120	ILE	C-N-CA	5.58	125.26	119.56
1	C	54	GLU	N-CA-C	5.58	117.81	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	VAL	N-CA-C	5.55	116.32	110.72
1	D	14	GLU	N-CA-C	5.50	119.94	113.23
1	A	73	THR	CA-C-N	5.49	125.01	119.19
1	A	73	THR	C-N-CA	5.49	125.01	119.19
1	B	251	ILE	N-CA-C	5.48	116.21	110.62
1	G	213	LEU	N-CA-C	-5.45	106.76	113.41
1	C	225	GLN	N-CA-C	5.43	118.73	111.24
1	H	254	SER	N-CA-C	-5.43	106.50	113.23
1	F	20	ASN	CA-C-N	5.42	128.47	120.82
1	F	20	ASN	C-N-CA	5.42	128.47	120.82
1	F	119	ILE	CB-CA-C	-5.42	104.92	112.02
1	D	152	PHE	CA-C-N	5.41	125.35	119.78
1	D	152	PHE	C-N-CA	5.41	125.35	119.78
1	E	85	THR	N-CA-CB	-5.40	102.50	110.49
1	G	123	VAL	N-CA-CB	5.39	117.47	110.57
1	C	197	VAL	CA-C-N	-5.38	114.05	120.13
1	C	197	VAL	C-N-CA	-5.38	114.05	120.13
1	E	321	THR	N-CA-C	-5.37	105.53	111.71
1	H	235	ASP	N-CA-C	5.36	118.04	111.82
1	F	114	ASN	N-CA-C	5.33	118.01	111.82
1	A	17	VAL	CB-CA-C	-5.33	104.66	110.37
1	A	111	ARG	N-CA-C	-5.33	104.90	111.40
1	F	52	VAL	N-CA-C	5.32	117.74	111.09
1	B	14	GLU	N-CA-C	5.32	116.97	108.41
1	B	80[A]	LYS	N-CA-C	-5.32	105.53	112.23
1	B	80[B]	LYS	N-CA-C	-5.32	105.53	112.23
1	C	290	VAL	N-CA-CB	-5.29	103.80	111.21
1	B	214	HIS	CA-C-N	5.29	126.45	119.84
1	B	214	HIS	C-N-CA	5.29	126.45	119.84
1	C	328	GLU	CB-CA-C	-5.29	104.71	111.22
1	B	75	LYS	N-CA-C	5.28	117.21	108.13
1	C	207	GLY	CA-C-N	-5.28	115.78	122.43
1	C	207	GLY	C-N-CA	-5.28	115.78	122.43
1	B	275	MET	CA-C-N	-5.27	114.29	122.67
1	B	275	MET	C-N-CA	-5.27	114.29	122.67
1	G	290	VAL	N-CA-C	-5.27	97.50	108.88
1	E	315	LEU	N-CA-C	-5.26	104.80	111.11
1	C	96	GLY	N-CA-C	5.25	118.26	110.60
1	B	276	LEU	N-CA-C	5.25	118.99	112.59
1	C	106	LEU	N-CA-C	-5.24	106.73	113.23
1	F	52	VAL	CB-CA-C	-5.23	103.78	112.26
1	G	200	TRP	N-CA-C	-5.23	105.64	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	68	SER	N-CA-C	5.22	117.71	111.71
1	E	136	SER	N-CA-C	5.21	117.79	110.23
1	H	299	ILE	CB-CA-C	-5.17	106.78	112.68
1	B	225	GLN	N-CA-C	5.16	118.36	111.24
1	E	198	PRO	N-CA-C	-5.16	101.85	112.47
1	G	221	ALA	N-CA-C	5.16	121.78	110.80
1	H	299	ILE	N-CA-C	5.15	114.01	106.55
1	A	68	SER	N-CA-C	5.14	116.89	111.28
1	E	270	HIS	CA-C-N	-5.14	113.41	119.84
1	E	270	HIS	C-N-CA	-5.14	113.41	119.84
1	E	14	GLU	N-CA-C	5.14	121.75	110.80
1	A	162	CYS	N-CA-C	-5.14	107.18	112.93
1	G	299	ILE	N-CA-CB	-5.11	105.23	111.21
1	C	126	TYR	CA-CB-CG	-5.09	104.73	113.90
1	B	282	ILE	N-CA-C	5.04	115.84	108.53
1	E	141	ILE	CB-CA-C	-5.02	105.29	112.22
1	E	143	THR	N-CA-C	-5.02	105.72	111.14
1	C	104	SER	N-CA-C	5.02	117.58	110.50
1	A	208	VAL	N-CA-C	5.01	114.82	107.15

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	13	LYS	Peptide
1	D	282	ILE	Peptide

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	2562	0	2644	208	0
1	B	2568	0	2655	130	0
1	C	2559	0	2639	190	0
1	D	2575	0	2653	182	0
1	E	2564	0	2643	208	0
1	F	2563	0	2644	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2571	0	2647	152	0
1	H	2568	0	2648	208	0
2	A	44	0	27	4	0
2	B	44	0	27	2	0
2	C	44	0	27	4	0
2	D	44	0	27	13	0
2	E	44	0	27	9	0
2	F	44	0	27	4	0
2	G	44	0	27	2	0
2	H	44	0	27	1	0
3	A	6	0	2	1	0
3	B	6	0	2	0	0
3	C	6	0	2	1	0
3	D	6	0	2	0	0
3	E	6	0	2	1	0
3	F	6	0	2	3	0
3	G	6	0	2	1	0
3	H	6	0	2	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	8	0	6	2	0
4	D	20	0	15	2	0
4	E	20	0	15	1	0
4	F	8	0	6	1	0
4	G	12	0	9	0	0
4	H	16	0	12	0	0
5	A	146	0	0	24	0
5	B	202	0	0	18	0
5	C	143	0	0	13	0
5	D	139	0	0	21	0
5	E	116	0	0	27	0
5	F	153	0	0	17	0
5	G	158	0	0	23	0
5	H	139	0	0	21	0
All	All	22218	0	21474	1381	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1381) 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:E:317:LYS:HZ2	1:E:317:LYS:CB	0.91	1.46
1:C:223:LYS:H	1:C:223:LYS:CD	1.25	1.45
1:A:106:LEU:O	1:A:106:LEU:HD23	1.26	1.28
1:H:308:THR:CG2	1:H:310:GLU:HG2	1.62	1.28
1:E:100:GLN:CG	1:E:101:GLU:H	1.42	1.27
1:H:219:THR:HG22	1:H:220:ASP:N	1.54	1.20
1:C:223:LYS:HD2	1:C:223:LYS:N	1.52	1.19
1:B:318:SER:O	1:B:322:LEU:HD23	1.43	1.19
1:B:225:GLN:HG2	5:B:613:HOH:O	1.38	1.18
1:A:317:LYS:HB2	1:A:317:LYS:NZ	1.32	1.16
1:E:100:GLN:HG2	1:E:101:GLU:N	1.43	1.15
1:H:308:THR:HG21	1:H:310:GLU:HG2	1.25	1.15
1:E:317:LYS:HB3	1:E:317:LYS:NZ	0.92	1.15
1:D:314:HIS:HB3	5:D:1072:HOH:O	1.44	1.14
1:G:9:HIS:HD2	5:G:1043:HOH:O	1.30	1.14
1:E:29:ALA:HB1	1:E:248:THR:HG21	1.26	1.12
1:A:111:ARG:HG2	1:A:111:ARG:HH11	1.12	1.12
1:C:327:LYS:N	1:C:327:LYS:HE3	1.63	1.11
1:B:56:LYS:HD2	5:B:1139:HOH:O	1.47	1.11
1:F:72:ARG:HH11	1:F:72:ARG:HG2	1.00	1.10
1:G:154:LYS:HE2	5:G:1150:HOH:O	1.49	1.10
1:F:141:ILE:CD1	1:F:325:ILE:HG21	1.81	1.09
1:E:105:ARG:HG3	1:E:108:LEU:HD23	1.21	1.09
1:H:308:THR:HB	1:H:311:GLU:HG3	1.35	1.09
1:C:3:LEU:HD21	1:D:210:LEU:HG	1.32	1.09
1:B:7:LEU:HG	1:B:8:ILE:HD12	1.33	1.08
1:C:246:TYR:CE2	1:C:248:THR:HG21	1.89	1.08
1:C:276:LEU:HD12	1:C:276:LEU:H	1.16	1.07
1:F:72:ARG:HH11	1:F:72:ARG:CG	1.64	1.06
1:B:29:ALA:HB1	1:B:248:THR:HG21	1.33	1.06
1:C:246:TYR:CE2	1:C:248:THR:CG2	2.39	1.05
1:D:135:VAL:O	2:D:332:NAI:H2N	1.56	1.05
1:D:170:ARG:HD3	1:D:184:CYS:O	1.56	1.05
1:A:317:LYS:HZ2	1:A:317:LYS:CB	1.69	1.05
1:E:14:GLU:HG3	1:E:14:GLU:O	1.50	1.04
1:C:283:LYS:HE3	1:C:283:LYS:HA	1.38	1.04
1:F:29:ALA:HB1	1:F:248:THR:CG2	1.88	1.03
1:F:276:LEU:HD12	1:F:276:LEU:H	1.22	1.03
1:A:228:GLN:OE1	1:A:228:GLN:HA	1.52	1.02
1:C:225:GLN:HG2	5:C:952:HOH:O	1.59	1.01
1:A:29:ALA:HB1	1:A:248:THR:HG21	1.42	1.00
1:A:227:LYS:HG3	5:A:1184:HOH:O	1.59	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LYS:H	1:C:327:LYS:CE	1.73	1.00
1:H:82:TYR:O	1:H:85:THR:HB	1.61	1.00
1:H:219:THR:CG2	1:H:220:ASP:H	1.74	1.00
1:C:327:LYS:HE3	1:C:327:LYS:H	0.86	1.00
1:H:99:GLN:NE2	1:H:103:GLU:HB2	1.75	1.00
1:E:225:GLN:HG3	1:E:228:GLN:HG2	1.44	0.99
1:A:82:TYR:O	1:A:85:THR:HB	1.63	0.99
1:H:317:LYS:NZ	1:H:317:LYS:HB3	1.75	0.99
1:B:276:LEU:HD12	1:B:276:LEU:H	1.25	0.98
1:A:103:GLU:OE1	1:A:104:SER:O	1.82	0.98
1:G:204:ASN:HA	1:G:210:LEU:CD1	1.93	0.98
1:C:246:TYR:CD2	1:C:248:THR:CG2	2.47	0.97
1:A:204:ASN:HA	1:A:210:LEU:CD1	1.95	0.97
1:C:110:GLN:HG3	5:C:630:HOH:O	1.62	0.97
1:C:223:LYS:H	1:C:223:LYS:HD2	0.82	0.97
1:C:246:TYR:HE2	1:C:248:THR:HG21	1.25	0.97
1:H:308:THR:HG22	1:H:310:GLU:HG2	1.43	0.97
1:C:223:LYS:H	1:C:223:LYS:CE	1.78	0.96
1:E:14:GLU:O	1:E:14:GLU:CG	2.13	0.96
1:A:215:PRO:HD2	5:A:965:HOH:O	1.65	0.96
1:G:29:ALA:HB1	1:G:248:THR:CG2	1.94	0.96
1:A:317:LYS:NZ	1:A:317:LYS:CB	2.19	0.95
1:G:82:TYR:O	1:G:85:THR:HB	1.65	0.95
1:H:99:GLN:CD	1:H:103:GLU:HB2	1.92	0.95
1:A:106:LEU:HD23	1:A:106:LEU:C	1.91	0.95
1:A:278:GLY:C	1:A:279:LEU:HD23	1.92	0.95
1:F:53[A]:MET:HE1	1:F:56:LYS:HZ2	1.28	0.94
1:H:163:ASN:HB3	5:H:351:HOH:O	1.67	0.94
1:E:237:ALA:O	1:E:241:ILE:HG13	1.66	0.94
1:H:100:GLN:HE21	1:H:111:ARG:NH2	1.65	0.94
1:H:188:ILE:O	1:H:189:LEU:HD12	1.68	0.94
1:B:29:ALA:HB1	1:B:248:THR:CG2	1.98	0.94
1:F:97:ALA:H	1:F:112:ASN:HD21	1.11	0.94
1:G:14:GLU:HB3	5:G:521:HOH:O	1.65	0.94
1:C:14:GLU:OE1	1:C:14:GLU:HA	1.67	0.94
1:E:105:ARG:CG	1:E:108:LEU:HD23	1.97	0.94
1:A:211:LYS:O	1:A:215:PRO:HA	1.68	0.94
1:H:219:THR:CG2	1:H:220:ASP:N	2.25	0.94
1:G:89:LYS:HE2	5:G:342:HOH:O	1.68	0.93
1:C:97:ALA:H	1:C:112:ASN:HD21	1.04	0.93
1:H:219:THR:HG22	1:H:221:ALA:H	1.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:LYS:CD	1:C:223:LYS:N	2.09	0.93
1:D:51:ASP:OD1	2:D:332:NAI:H1B	1.67	0.93
1:H:219:THR:HG22	1:H:220:ASP:H	1.17	0.93
1:F:72:ARG:HG2	1:F:72:ARG:NH1	1.82	0.92
1:H:170:ARG:HD3	1:H:184:CYS:O	1.70	0.92
1:A:103:GLU:CD	1:A:104:SER:N	2.27	0.92
1:E:82:TYR:O	1:E:85:THR:HB	1.69	0.92
1:E:317:LYS:HB3	1:E:317:LYS:HZ3	1.16	0.91
1:B:323:TRP:HE1	1:B:327:LYS:HE3	1.35	0.91
1:D:117:LYS:HE3	1:D:331:PHE:C	1.96	0.91
1:F:141:ILE:HD13	1:F:325:ILE:HG21	1.51	0.91
1:E:317:LYS:HZ2	1:E:317:LYS:HB2	1.31	0.91
1:B:97:ALA:H	1:B:112:ASN:HD21	1.12	0.91
1:F:16:HIS:H	4:F:335:ACT:H3	1.32	0.91
1:D:136:SER:HA	2:D:332:NAI:H1D	1.53	0.90
1:F:29:ALA:HB1	1:F:248:THR:HG21	1.50	0.90
1:F:141:ILE:HD13	1:F:325:ILE:CG2	2.01	0.90
1:C:3:LEU:HD13	1:D:214:HIS:HB2	1.52	0.90
1:H:317:LYS:HB3	1:H:317:LYS:HZ3	1.34	0.90
1:A:198:PRO:HG3	1:A:230:HIS:CG	2.07	0.90
1:A:106:LEU:O	1:A:106:LEU:CD2	2.17	0.89
1:B:18:PRO:HB3	1:B:46:GLU:OE2	1.72	0.89
1:E:219:THR:CG2	1:E:221:ALA:H	1.84	0.89
1:A:110:GLN:O	1:A:110:GLN:HG3	1.71	0.89
1:G:211:LYS:HB3	5:G:483:HOH:O	1.70	0.89
1:C:276:LEU:HD12	1:C:276:LEU:N	1.75	0.89
1:D:308:THR:HG22	1:D:311:GLU:H	1.37	0.89
1:H:29:ALA:HB1	1:H:248:THR:CG2	2.03	0.88
1:B:322:LEU:O	1:B:326:GLN:HG3	1.74	0.88
1:C:325:ILE:HG22	1:C:325:ILE:O	1.72	0.88
1:C:82:TYR:O	1:C:85:THR:HB	1.75	0.87
1:H:99:GLN:HG3	1:H:100:GLN:O	1.75	0.87
1:B:7:LEU:CG	1:B:8:ILE:HD12	2.03	0.87
1:C:144:TYR:OH	1:C:148:LYS:HE3	1.73	0.87
1:G:214:HIS:HB2	1:H:3:LEU:HD13	1.57	0.86
1:A:216:GLU:OE2	1:A:223:LYS:CD	2.23	0.86
1:A:111:ARG:HG2	1:A:111:ARG:NH1	1.87	0.86
1:G:323:TRP:O	1:G:327:LYS:HG3	1.75	0.86
1:G:324:GLY:O	1:G:327:LYS:HD2	1.76	0.86
1:D:82:TYR:O	1:D:85:THR:HB	1.75	0.86
1:H:99:GLN:HE21	1:H:103:GLU:HG3	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:ASP:HB2	5:G:473:HOH:O	1.74	0.85
1:E:263:MET:HE3	5:E:524:HOH:O	1.74	0.85
1:F:14:GLU:OE2	1:F:16:HIS:HB2	1.75	0.85
1:G:97:ALA:H	1:G:112:ASN:HD21	1.22	0.85
1:H:317:LYS:HE2	5:H:852:HOH:O	1.75	0.85
1:C:15:GLU:O	1:C:15:GLU:HG2	1.77	0.84
1:B:276:LEU:HD12	1:B:276:LEU:N	1.89	0.84
1:A:204:ASN:HA	1:A:210:LEU:HD11	1.56	0.84
1:H:229:VAL:O	1:H:233:VAL:HG23	1.78	0.84
1:H:308:THR:HG21	1:H:310:GLU:CG	2.06	0.84
1:A:103:GLU:CD	1:A:103:GLU:C	2.43	0.84
1:H:284:GLU:HG2	1:H:316:LYS:NZ	1.93	0.84
1:H:162:CYS:HA	1:H:165:ASP:OD1	1.78	0.84
1:D:29:ALA:HB1	1:D:248:THR:CG2	2.07	0.84
1:H:326:GLN:HA	1:H:329:LEU:HD23	1.58	0.84
1:D:10:ASN:HD21	1:D:13:LYS:HG3	1.43	0.84
1:E:27:VAL:HG11	1:E:57:LEU:HD12	1.60	0.83
1:G:120:ILE:O	1:G:124:VAL:HG13	1.78	0.83
1:B:15:GLU:CD	1:B:15:GLU:H	1.85	0.83
1:E:29:ALA:CB	1:E:248:THR:HG21	2.06	0.83
1:H:219:THR:CG2	1:H:221:ALA:H	1.91	0.83
1:B:82:TYR:O	1:B:85:THR:HB	1.77	0.83
1:F:29:ALA:HB1	1:F:248:THR:HG22	1.60	0.83
1:F:53[A]:MET:HE1	1:F:56:LYS:NZ	1.93	0.83
1:C:317:LYS:HB3	1:C:317:LYS:HZ2	1.44	0.83
1:F:60:GLU:OE1	1:F:60:GLU:HA	1.79	0.83
1:C:246:TYR:HE2	1:C:248:THR:CG2	1.84	0.82
5:E:794:HOH:O	1:F:53[B]:MET:HE2	1.78	0.82
1:H:99:GLN:NE2	1:H:103:GLU:HG3	1.93	0.82
1:A:120:ILE:O	1:A:124:VAL:HG13	1.79	0.82
1:A:317:LYS:HE3	1:A:317:LYS:C	2.05	0.82
1:E:105:ARG:NE	1:E:108:LEU:HD22	1.94	0.82
1:H:188:ILE:C	1:H:189:LEU:CD1	2.53	0.82
1:F:204:ASN:HA	1:F:210:LEU:HD13	1.60	0.82
1:D:176:ARG:HH21	1:D:229:VAL:CG2	1.92	0.81
1:G:61:MET:O	1:G:65:GLN:HG3	1.80	0.81
1:B:246:TYR:CD2	1:B:248:THR:HG23	2.15	0.81
1:B:7:LEU:CD2	1:B:8:ILE:CD1	2.58	0.81
1:F:99:GLN:HG3	5:F:395:HOH:O	1.80	0.81
1:E:200:TRP:HA	1:E:203:MET:HE3	1.62	0.81
1:G:29:ALA:HB1	1:G:248:THR:HG21	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:356:HOH:O	1:F:53[B]:MET:HE3	1.81	0.81
1:F:109:VAL:CG1	1:F:138:PRO:HG2	2.11	0.81
1:E:169:PHE:HD2	1:E:233:VAL:HG21	1.46	0.80
1:E:13:LYS:NZ	1:E:13:LYS:HB3	1.95	0.80
1:E:170:ARG:NH2	1:F:69:LEU:HD11	1.95	0.80
1:E:200:TRP:CE3	1:E:203:MET:HE1	2.16	0.80
1:B:32:MET:HE1	1:B:64:LEU:HD11	1.62	0.80
1:G:120:ILE:O	1:G:124:VAL:CG1	2.29	0.80
1:D:316:LYS:HD2	4:D:336:ACT:C	2.11	0.80
1:F:141:ILE:CD1	1:F:325:ILE:CG2	2.59	0.80
1:H:106:LEU:CD2	1:H:328:GLU:OE1	2.30	0.79
1:G:231:LYS:HG2	5:G:1009:HOH:O	1.81	0.79
1:C:276:LEU:HD13	1:C:276:LEU:C	2.05	0.79
1:E:130:CYS:O	1:E:156:ARG:HD2	1.82	0.79
1:C:325:ILE:O	1:C:325:ILE:CG2	2.31	0.79
1:H:188:ILE:C	1:H:189:LEU:HD12	2.07	0.79
1:A:29:ALA:HB1	1:A:248:THR:CG2	2.13	0.79
1:H:327:LYS:HB3	1:H:327:LYS:HZ3	1.47	0.79
1:A:100:GLN:HB2	1:A:111:ARG:HH22	1.48	0.78
1:E:219:THR:HG22	1:E:221:ALA:H	1.46	0.78
1:A:216:GLU:OE2	1:A:223:LYS:HD3	1.83	0.78
1:A:317:LYS:HE3	1:A:317:LYS:O	1.82	0.78
1:C:129:HIS:HB2	4:C:334:ACT:H2	1.66	0.78
1:D:29:ALA:O	1:D:248:THR:HG22	1.84	0.78
1:H:170:ARG:CD	1:H:184:CYS:O	2.30	0.78
1:G:204:ASN:HA	1:G:210:LEU:HD13	1.64	0.78
1:H:308:THR:CG2	1:H:310:GLU:CG	2.55	0.78
1:A:228:GLN:OE1	1:A:228:GLN:CA	2.32	0.78
1:H:99:GLN:NE2	1:H:103:GLU:CB	2.46	0.77
1:H:326:GLN:HA	1:H:329:LEU:CD2	2.14	0.77
1:F:283:LYS:HD2	1:F:283:LYS:N	1.98	0.77
1:A:105:ARG:NH1	1:A:108:LEU:CD2	2.47	0.77
1:H:327:LYS:CB	1:H:327:LYS:NZ	2.47	0.77
1:H:277:LYS:HE3	1:H:285:ASP:OD2	1.85	0.77
1:D:135:VAL:O	2:D:332:NAI:C2N	2.31	0.77
1:C:223:LYS:N	1:C:223:LYS:CE	2.43	0.77
1:E:99:GLN:HB3	1:E:111:ARG:HG3	1.66	0.77
1:F:246:TYR:CD2	1:F:248:THR:HG23	2.20	0.77
1:H:219:THR:HG22	1:H:221:ALA:N	2.00	0.76
1:F:192:HIS:CD2	1:F:192:HIS:O	2.39	0.76
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:LEU:HD22	1:H:328:GLU:OE1	1.85	0.76
1:G:276:LEU:HD13	1:G:276:LEU:C	2.09	0.76
5:E:354:HOH:O	1:H:11:LEU:HD23	1.86	0.76
1:A:277:LYS:HD3	1:A:285:ASP:OD2	1.86	0.76
1:B:169:PHE:CE1	1:B:173:MET:HE2	2.21	0.76
1:A:222:ASP:CG	1:A:224:GLU:O	2.29	0.75
1:C:276:LEU:C	1:C:276:LEU:CD1	2.59	0.75
1:D:316:LYS:HD2	4:D:336:ACT:OXT	1.86	0.75
1:B:85:THR:CG2	5:B:1140:HOH:O	2.34	0.75
1:C:14:GLU:OE1	1:C:14:GLU:CA	2.34	0.75
1:E:317:LYS:CB	1:E:317:LYS:NZ	1.76	0.75
1:B:7:LEU:CD2	1:B:8:ILE:HD12	2.16	0.75
1:C:65:GLN:O	1:C:68:SER:HB3	1.87	0.75
1:E:100:GLN:HG2	1:E:101:GLU:H	0.63	0.75
1:B:246:TYR:HD2	1:B:248:THR:HG23	1.52	0.75
1:C:246:TYR:HD2	1:C:248:THR:CG2	2.00	0.75
1:C:170:ARG:HD3	1:C:184:CYS:O	1.86	0.75
1:C:246:TYR:CD2	1:C:248:THR:HG23	2.22	0.75
2:A:332:NAI:H42N	3:A:333:OXM:C1	2.16	0.74
1:C:170:ARG:CD	1:C:184:CYS:O	2.34	0.74
1:F:239:GLU:HG3	5:F:450:HOH:O	1.85	0.74
1:H:215:PRO:HD2	1:H:216:GLU:OE2	1.87	0.74
1:E:99:GLN:HB2	1:E:111:ARG:HH11	1.50	0.74
1:G:124:VAL:HG23	1:G:124:VAL:O	1.86	0.74
1:H:99:GLN:CD	1:H:103:GLU:CB	2.60	0.74
1:H:151:GLY:HA2	5:H:347:HOH:O	1.87	0.74
1:C:317:LYS:HB3	1:C:317:LYS:NZ	2.02	0.74
1:A:216:GLU:O	1:A:219:THR:HB	1.88	0.74
1:C:246:TYR:CE2	1:C:248:THR:HG23	2.21	0.74
1:E:251:ILE:HG12	2:E:332:NAI:H4N	1.70	0.74
1:B:80[A]:LYS:HG2	5:B:414:HOH:O	1.88	0.74
1:D:25:VAL:HA	1:D:50[B]:VAL:HG23	1.68	0.74
1:D:29:ALA:HB1	1:D:248:THR:HG23	1.68	0.74
1:E:187:TRP:HB2	5:E:378:HOH:O	1.87	0.74
1:E:308:THR:OG1	1:E:311:GLU:HG3	1.87	0.73
1:D:216:GLU:O	1:D:222:ASP:HB2	1.88	0.73
1:E:25:VAL:HG13	1:E:50:VAL:HG22	1.70	0.73
1:A:105:ARG:NH1	1:A:108:LEU:HD23	2.03	0.73
5:G:697:HOH:O	1:H:2:ALA:HB1	1.89	0.73
1:H:29:ALA:HB1	1:H:248:THR:HG21	1.69	0.73
1:H:227:LYS:HD3	5:H:712:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:PRO:HD3	1:C:230:HIS:CE1	2.24	0.73
1:E:314:HIS:CE1	5:E:441:HOH:O	2.42	0.73
1:F:194:ASP:N	1:F:194:ASP:OD1	2.19	0.73
1:F:276:LEU:HD12	1:F:276:LEU:N	1.87	0.73
1:H:248:THR:CB	5:H:705:HOH:O	2.35	0.73
1:H:284:GLU:CG	1:H:316:LYS:HZ2	2.01	0.73
1:E:225:GLN:CG	1:E:228:GLN:HG2	2.18	0.72
1:A:105:ARG:HH11	1:A:105:ARG:CG	2.01	0.72
1:B:97:ALA:N	1:B:112:ASN:HD21	1.86	0.72
1:H:284:GLU:HG2	1:H:316:LYS:HZ2	1.54	0.72
1:C:323:TRP:HA	1:C:323:TRP:CE3	2.24	0.72
1:A:216:GLU:HG3	1:A:222:ASP:OD1	1.90	0.72
1:B:106:LEU:O	1:B:109:VAL:HG12	1.90	0.72
1:H:308:THR:HB	1:H:311:GLU:CG	2.16	0.72
1:B:9:HIS:HB2	1:C:304:LYS:HD2	1.72	0.72
1:B:16:HIS:N	1:B:16:HIS:CD2	2.58	0.72
1:B:180:HIS:CE1	1:B:182:LEU:HD22	2.25	0.72
1:C:284:GLU:OE1	1:C:284:GLU:N	2.24	0.71
1:E:105:ARG:O	1:E:109:VAL:HG23	1.90	0.71
1:F:140:ASP:HB2	5:F:509:HOH:O	1.89	0.71
1:E:99:GLN:OE1	1:E:99:GLN:C	2.34	0.71
1:D:117:LYS:HE3	1:D:331:PHE:O	1.89	0.71
1:C:323:TRP:HA	1:C:323:TRP:HE3	1.56	0.71
1:F:110:GLN:HB2	5:F:362:HOH:O	1.89	0.71
1:H:308:THR:HG22	1:H:310:GLU:H	1.53	0.71
1:D:17:VAL:HG22	5:D:363:HOH:O	1.89	0.71
1:F:330:GLN:CD	1:F:330:GLN:H	1.98	0.71
1:H:189:LEU:CD1	1:H:189:LEU:N	2.54	0.71
1:B:8:ILE:HG23	1:C:301:ASP:HB3	1.73	0.70
1:D:104:SER:OG	1:D:105:ARG:N	2.22	0.70
1:C:97:ALA:N	1:C:112:ASN:HD21	1.86	0.70
1:F:141:ILE:HD11	1:F:325:ILE:HG21	1.72	0.70
1:G:56:LYS:CG	5:G:353:HOH:O	2.39	0.70
1:A:103:GLU:OE1	1:A:107:ASN:HB3	1.92	0.70
1:A:214:HIS:CE1	5:A:964:HOH:O	2.44	0.70
1:G:29:ALA:HB1	1:G:248:THR:HG23	1.71	0.70
1:G:276:LEU:HD12	1:G:276:LEU:H	1.54	0.70
1:B:16:HIS:HB3	5:B:914:HOH:O	1.91	0.70
1:G:56:LYS:HG2	5:G:353:HOH:O	1.90	0.69
1:H:151:GLY:C	5:H:347:HOH:O	2.34	0.69
1:H:16:HIS:CE1	5:H:955:HOH:O	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:ASP:O	1:H:74:PRO:HD2	1.92	0.69
1:H:327:LYS:HB3	1:H:327:LYS:NZ	2.06	0.69
1:A:2:ALA:HA	1:B:224:GLU:OE2	1.93	0.69
1:C:324:GLY:C	1:C:327:LYS:NZ	2.51	0.69
1:E:99:GLN:OE1	1:E:99:GLN:O	2.11	0.69
1:G:3:LEU:HD13	1:H:214:HIS:HB2	1.74	0.69
1:H:99:GLN:NE2	1:H:103:GLU:CG	2.56	0.69
1:F:237:ALA:O	1:F:241:ILE:HG13	1.92	0.69
1:H:29:ALA:HB1	1:H:248:THR:HG23	1.75	0.69
1:H:151:GLY:CA	5:H:347:HOH:O	2.41	0.68
1:D:30:VAL:HG21	2:D:332:NAI:H52N	1.74	0.68
1:E:219:THR:HG23	1:E:221:ALA:H	1.58	0.68
1:F:304:LYS:HD2	1:G:9:HIS:HB2	1.75	0.68
1:B:169:PHE:CE1	1:B:173:MET:CE	2.76	0.68
1:C:238:TYR:HB2	5:C:899:HOH:O	1.93	0.68
1:H:242:LYS:CG	1:H:242:LYS:O	2.41	0.68
1:B:323:TRP:NE1	1:B:327:LYS:HE3	2.07	0.68
1:E:282:ILE:HD13	1:E:282:ILE:N	2.06	0.68
1:G:276:LEU:C	1:G:276:LEU:CD1	2.66	0.68
1:E:314:HIS:HB3	5:E:538:HOH:O	1.93	0.68
1:H:308:THR:HG22	1:H:310:GLU:N	2.08	0.68
1:A:111:ARG:O	1:A:114:ASN:HB2	1.93	0.68
1:H:188:ILE:C	1:H:189:LEU:HD13	2.18	0.68
1:H:180:HIS:CE1	1:H:182:LEU:HD22	2.29	0.68
1:A:129:HIS:NE2	5:A:1155:HOH:O	2.27	0.67
1:B:14:GLU:CG	5:B:968:HOH:O	2.42	0.67
1:E:219:THR:HG22	1:E:222:ASP:H	1.59	0.67
1:C:308:THR:O	1:C:312:GLU:HB2	1.93	0.67
1:D:320:ASP:CB	5:D:953:HOH:O	2.41	0.67
1:G:75:LYS:HD3	5:G:355:HOH:O	1.93	0.67
1:B:131:LYS:NZ	1:B:296:GLN:O	2.23	0.67
1:G:231:LYS:CG	5:G:1009:HOH:O	2.39	0.67
1:E:85:THR:CG2	5:E:348:HOH:O	2.42	0.67
1:H:16:HIS:HE1	5:H:955:HOH:O	1.75	0.67
1:G:219:THR:HG22	1:G:220:ASP:N	2.10	0.67
1:A:203:MET:O	1:A:210:LEU:HD13	1.94	0.67
1:C:13:LYS:CG	1:C:13:LYS:O	2.43	0.67
1:D:176:ARG:NH2	1:D:229:VAL:CG2	2.57	0.67
1:E:46:GLU:CD	1:E:75:LYS:HD3	2.20	0.67
1:F:326:GLN:HB2	1:F:329:LEU:HD22	1.77	0.67
1:H:284:GLU:CG	1:H:316:LYS:NZ	2.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:GLU:O	1:E:101:GLU:HG2	1.95	0.67
1:F:246:TYR:HD2	1:F:248:THR:HG23	1.59	0.67
1:A:314:HIS:O	1:A:317:LYS:HG3	1.95	0.66
1:F:200:TRP:CH2	1:F:227:LYS:HA	2.30	0.66
1:H:103:GLU:O	1:H:103:GLU:HG2	1.93	0.66
1:A:276:LEU:HD12	1:A:276:LEU:H	1.58	0.66
1:F:179:VAL:HG12	1:F:180:HIS:N	2.11	0.66
1:A:135:VAL:O	2:A:332:NAI:H2N	1.95	0.66
1:B:16:HIS:CE1	5:B:749:HOH:O	2.49	0.66
1:B:85:THR:HG22	5:B:1140:HOH:O	1.93	0.66
1:B:21:LYS:HB3	1:B:88:SER:HA	1.78	0.66
1:E:25:VAL:HG13	1:E:50:VAL:CG2	2.26	0.66
1:H:329:LEU:HB3	1:H:331:PHE:HD2	1.60	0.66
1:C:283:LYS:HE3	1:C:283:LYS:CA	2.18	0.66
1:B:9:HIS:HB2	1:C:304:LYS:CD	2.26	0.66
1:B:277:LYS:HE2	1:B:285:ASP:OD1	1.95	0.66
1:F:170:ARG:HD2	1:F:184:CYS:O	1.96	0.66
1:A:85:THR:CG2	5:A:346:HOH:O	2.43	0.66
1:A:218:GLY:O	1:A:227:LYS:HD2	1.95	0.66
1:C:2:ALA:HA	1:D:224:GLU:OE1	1.96	0.66
1:E:159:GLY:HA3	1:E:273:SER:HB3	1.78	0.66
1:B:14:GLU:HG3	5:B:968:HOH:O	1.96	0.66
1:C:13:LYS:O	1:C:13:LYS:HD2	1.96	0.66
1:E:29:ALA:HB1	1:E:248:THR:CG2	2.14	0.66
1:F:187:TRP:CZ3	1:F:271:PRO:HB3	2.31	0.66
1:H:100:GLN:NE2	1:H:111:ARG:NH2	2.40	0.66
1:A:17:VAL:HG12	1:A:17:VAL:O	1.95	0.66
1:A:75:LYS:HG3	5:D:971:HOH:O	1.96	0.66
1:B:204:ASN:HD22	1:B:207:GLY:H	1.43	0.66
1:G:85:THR:CG2	5:G:468:HOH:O	2.44	0.66
1:C:324:GLY:CA	1:C:327:LYS:HZ1	2.09	0.65
1:F:109:VAL:HG13	1:F:138:PRO:HG2	1.78	0.65
1:F:162:CYS:HA	1:F:165:ASP:OD1	1.95	0.65
1:A:210:LEU:N	1:A:210:LEU:HD12	2.12	0.65
1:G:204:ASN:CA	1:G:210:LEU:HD13	2.26	0.65
1:C:50:VAL:HB	1:C:79:GLY:O	1.97	0.65
1:E:163:ASN:HD22	1:E:254:SER:HB2	1.61	0.65
1:E:170:ARG:NH2	1:F:69:LEU:CD1	2.59	0.65
1:F:14:GLU:OE2	1:F:16:HIS:CB	2.45	0.65
1:F:246:TYR:CE2	1:F:248:THR:CG2	2.79	0.65
1:A:317:LYS:HB2	1:A:317:LYS:HZ2	0.73	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:LYS:HD3	1:F:46:GLU:HG2	1.77	0.65
1:G:204:ASN:CA	1:G:210:LEU:CD1	2.73	0.65
1:B:21:LYS:HE3	1:B:46:GLU:OE1	1.94	0.65
1:C:223:LYS:N	1:C:223:LYS:HE2	2.10	0.65
1:G:69:LEU:HD12	1:H:182:LEU:HD13	1.78	0.65
1:A:113:VAL:O	1:A:117:LYS:HG3	1.97	0.65
1:E:170:ARG:HD2	1:E:184:CYS:O	1.96	0.65
1:G:276:LEU:HD13	1:G:276:LEU:O	1.97	0.65
1:G:219:THR:CG2	1:G:220:ASP:N	2.60	0.65
1:A:103:GLU:OE2	1:A:104:SER:N	2.29	0.65
1:F:72:ARG:CG	1:F:72:ARG:NH1	2.38	0.65
1:D:176:ARG:HH21	1:D:229:VAL:HG22	1.59	0.65
1:F:321:THR:HG22	1:F:322:LEU:N	2.12	0.65
1:D:29:ALA:HB1	1:D:248:THR:HG21	1.77	0.64
1:H:277:LYS:HD2	1:H:283:LYS:O	1.97	0.64
1:E:13:LYS:O	1:E:15:GLU:HG2	1.98	0.64
1:H:120:ILE:HB	1:H:121:PRO:HD3	1.79	0.64
1:A:122:ASN:CG	5:A:552:HOH:O	2.39	0.64
1:D:235:ASP:O	1:D:239[B]:GLU:HG2	1.98	0.64
1:E:105:ARG:HG3	1:E:108:LEU:CD2	2.13	0.64
1:G:124:VAL:O	1:G:124:VAL:CG2	2.45	0.64
1:H:327:LYS:HZ2	1:H:327:LYS:HB2	1.63	0.64
1:D:321:THR:O	1:D:322:LEU:C	2.39	0.64
2:D:332:NAI:H6N	2:D:332:NAI:H51N	1.79	0.64
1:A:265:ASN:CG	1:A:296:GLN:HG2	2.23	0.64
1:A:326:GLN:HA	1:A:329:LEU:HD22	1.79	0.64
1:G:58:LYS:HG3	5:G:360:HOH:O	1.97	0.64
1:G:324:GLY:C	1:G:327:LYS:HD2	2.23	0.64
1:E:99:GLN:HA	1:E:111:ARG:NH1	2.12	0.64
1:E:215:PRO:HD2	5:E:367:HOH:O	1.97	0.64
1:E:180:HIS:CE1	1:E:182:LEU:CD2	2.81	0.64
1:D:2:ALA:O	1:D:6:GLN:HG3	1.97	0.63
1:E:316:LYS:HD2	1:E:316:LYS:C	2.24	0.63
1:F:81:ASP:C	1:F:81:ASP:OD1	2.40	0.63
1:C:13:LYS:O	1:C:13:LYS:HG3	1.97	0.63
1:C:275:MET:SD	1:C:277:LYS:HB3	2.38	0.63
1:H:328:GLU:O	1:H:329:LEU:C	2.40	0.63
1:B:7:LEU:HD23	1:B:8:ILE:CD1	2.27	0.63
1:G:13:LYS:C	1:G:13:LYS:CD	2.71	0.63
1:A:100:GLN:HB2	1:A:111:ARG:NH2	2.12	0.63
1:D:230:HIS:O	1:D:234:VAL:CG1	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:LYS:HE3	5:F:935:HOH:O	1.98	0.63
1:F:314:HIS:HB3	5:F:374:HOH:O	1.99	0.63
1:H:56:LYS:HE2	5:H:339:HOH:O	1.97	0.63
1:E:191:GLU:C	1:E:192:HIS:O	2.42	0.63
1:C:85:THR:O	1:C:85:THR:CG2	2.45	0.62
1:D:53:MET:CE	1:D:56:LYS:HD3	2.29	0.62
1:D:283:LYS:NZ	1:D:316:LYS:HG3	2.13	0.62
1:G:72:ARG:NH1	5:G:358:HOH:O	2.21	0.62
1:D:230:HIS:O	1:D:234:VAL:HG13	1.98	0.62
1:E:120:ILE:O	1:E:124:VAL:HG13	1.98	0.62
1:G:29:ALA:C	1:G:248:THR:HG22	2.25	0.62
1:G:324:GLY:O	1:G:327:LYS:CD	2.46	0.62
1:A:103:GLU:OE1	1:A:104:SER:C	2.42	0.62
1:E:223:LYS:HD2	1:E:223:LYS:C	2.25	0.62
1:H:317:LYS:HB3	1:H:317:LYS:HZ2	1.63	0.62
1:A:272:ILE:O	1:A:289:SER:HA	2.00	0.62
1:D:248:THR:HG21	5:D:559:HOH:O	1.99	0.62
1:E:81:ASP:OD2	1:E:83:SER:N	2.27	0.62
1:E:109:VAL:HG11	1:E:141:ILE:HG21	1.82	0.62
1:E:200:TRP:CE3	1:E:203:MET:CE	2.82	0.62
1:G:208:VAL:CG2	1:H:7:LEU:CD1	2.77	0.62
1:H:299:ILE:O	1:H:299:ILE:HG22	2.00	0.62
1:D:30:VAL:CG2	2:D:332:NAI:H52N	2.30	0.62
1:G:276:LEU:HD12	1:G:276:LEU:N	2.13	0.62
1:F:279:LEU:N	1:F:279:LEU:HD22	2.14	0.61
1:D:204:ASN:C	1:D:204:ASN:ND2	2.59	0.61
1:F:205:VAL:O	1:F:208:VAL:HG23	2.00	0.61
1:C:170:ARG:HD2	1:C:184:CYS:O	1.99	0.61
1:D:53:MET:HE3	1:D:56:LYS:HD3	1.83	0.61
1:D:308:THR:HG22	1:D:310:GLU:N	2.14	0.61
1:E:105:ARG:NE	1:E:108:LEU:CD2	2.63	0.61
1:H:29:ALA:C	1:H:248:THR:HG22	2.24	0.61
1:E:28:GLY:N	5:E:433:HOH:O	2.33	0.61
1:A:85:THR:HG22	5:A:346:HOH:O	2.00	0.61
1:A:276:LEU:HD12	1:A:276:LEU:N	2.15	0.61
1:B:15:GLU:CD	1:B:15:GLU:N	2.52	0.61
1:A:106:LEU:C	1:A:106:LEU:CD2	2.67	0.61
1:D:196:SER:OG	1:D:230:HIS:HE1	1.83	0.61
1:E:267:ARG:HA	1:E:294:LEU:O	2.01	0.61
1:A:216:GLU:OE2	1:A:223:LYS:HD2	2.01	0.61
1:C:180:HIS:CE1	1:C:182:LEU:HD22	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:LYS:C	1:E:223:LYS:CD	2.74	0.61
1:G:204:ASN:HD22	1:G:207:GLY:H	1.45	0.61
1:G:219:THR:HG22	1:G:221:ALA:N	2.15	0.61
1:G:237:ALA:O	1:G:241:ILE:HG13	2.00	0.61
1:H:188:ILE:O	1:H:189:LEU:CD1	2.44	0.61
1:D:320:ASP:HB3	5:D:953:HOH:O	2.01	0.61
1:H:187:TRP:CZ3	1:H:271:PRO:HD3	2.35	0.61
1:C:228:GLN:O	1:C:232:GLN:HG3	2.01	0.61
1:F:141:ILE:HD13	1:F:325:ILE:HG22	1.81	0.61
1:F:323:TRP:O	1:F:327:LYS:HB2	2.00	0.61
1:C:115:ILE:HD12	5:C:1160:HOH:O	2.01	0.60
1:D:308:THR:CG2	1:D:310:GLU:H	2.14	0.60
1:F:246:TYR:HE2	1:F:248:THR:HG21	1.66	0.60
1:C:267:ARG:HH11	1:C:267:ARG:HG2	1.66	0.60
1:E:328:GLU:HA	1:E:328:GLU:OE1	2.02	0.60
1:C:324:GLY:HA2	1:C:327:LYS:NZ	2.17	0.60
1:E:13:LYS:HB3	1:E:13:LYS:HZ2	1.67	0.60
1:E:28:GLY:C	5:E:428:HOH:O	2.44	0.60
1:E:191:GLU:O	1:E:192:HIS:O	2.19	0.60
1:A:108:LEU:C	1:A:108:LEU:HD12	2.25	0.60
1:D:170:ARG:CD	1:D:184:CYS:O	2.42	0.60
1:D:171:TYR:CD1	5:D:354:HOH:O	2.51	0.60
1:E:204:ASN:HA	1:E:210:LEU:HD13	1.84	0.60
1:B:216:GLU:O	1:B:217:LEU:C	2.45	0.60
1:B:246:TYR:CE2	1:B:248:THR:CG2	2.84	0.60
1:G:29:ALA:CB	1:G:248:THR:CG2	2.76	0.60
1:G:50:VAL:HB	1:G:79:GLY:O	2.01	0.60
1:G:201:SER:HA	1:G:211:LYS:HD2	1.84	0.60
1:A:219:THR:CG2	1:A:221:ALA:N	2.64	0.60
1:F:97:ALA:N	1:F:112:ASN:HD21	1.93	0.60
1:G:97:ALA:N	1:G:112:ASN:HD21	1.98	0.60
1:A:276:LEU:CD1	1:A:276:LEU:C	2.75	0.60
1:D:308:THR:HG22	1:D:311:GLU:N	2.15	0.60
1:C:131:LYS:HE3	1:C:296:GLN:O	2.01	0.59
1:H:27:VAL:HG22	1:H:51:ASP:OD2	2.02	0.59
1:H:29:ALA:O	1:H:248:THR:HG22	2.00	0.59
1:D:151:GLY:C	5:D:1125:HOH:O	2.45	0.59
1:F:246:TYR:CE2	1:F:248:THR:HG23	2.38	0.59
1:H:98:ARG:HD2	5:H:1171:HOH:O	2.01	0.59
1:H:106:LEU:HD11	1:H:325:ILE:HG23	1.84	0.59
1:A:100:GLN:O	1:A:103:GLU:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:GLU:O	1:C:15:GLU:CG	2.50	0.59
1:C:327:LYS:HD2	1:C:328:GLU:N	2.17	0.59
1:E:16:HIS:CG	1:E:16:HIS:O	2.55	0.59
1:A:317:LYS:C	1:A:317:LYS:CE	2.76	0.59
1:B:80[A]:LYS:HD2	5:B:384:HOH:O	2.00	0.59
1:F:18:PRO:HA	5:F:354:HOH:O	2.02	0.59
1:G:216:GLU:O	1:G:219:THR:HB	2.03	0.59
1:A:190:GLY:O	1:A:289:SER:HB2	2.02	0.59
1:D:283:LYS:HE3	1:D:316:LYS:HG3	1.84	0.59
1:A:219:THR:CG2	1:A:220:ASP:N	2.64	0.59
1:C:125:LYS:HD3	1:C:126:TYR:CE1	2.37	0.59
1:D:308:THR:CG2	1:D:310:GLU:N	2.66	0.59
1:E:8:ILE:CG2	1:E:9:HIS:N	2.65	0.59
1:A:219:THR:HG23	1:A:220:ASP:N	2.17	0.59
1:D:308:THR:HG23	1:D:310:GLU:H	1.67	0.59
1:G:75:LYS:HE3	1:G:77:VAL:CG1	2.32	0.59
1:H:248:THR:HG21	5:H:705:HOH:O	2.02	0.59
1:C:16:HIS:HE1	1:C:18:PRO:HA	1.68	0.59
1:E:32:MET:HE1	1:E:64:LEU:HD11	1.85	0.59
1:A:296:GLN:HE22	1:D:19:GLN:HG2	1.67	0.59
1:C:222:ASP:C	1:C:222:ASP:OD1	2.46	0.59
1:D:85:THR:CG2	1:D:85:THR:O	2.51	0.59
1:D:248:THR:O	1:D:251:ILE:HG22	2.03	0.59
1:E:219:THR:HG22	1:E:221:ALA:N	2.17	0.59
1:H:329:LEU:HB3	1:H:331:PHE:CD2	2.37	0.59
1:D:248:THR:O	1:D:251:ILE:CG2	2.51	0.58
1:F:246:TYR:CD2	1:F:248:THR:CG2	2.86	0.58
5:A:361:HOH:O	1:B:182:LEU:HD21	2.02	0.58
1:C:144:TYR:CZ	1:C:148:LYS:HE3	2.37	0.58
1:E:180:HIS:CE1	1:E:182:LEU:HD23	2.38	0.58
1:F:14:GLU:HB2	5:G:996:HOH:O	2.02	0.58
1:E:105:ARG:HE	1:E:108:LEU:HD22	1.68	0.58
1:G:208:VAL:HG22	1:H:7:LEU:HD11	1.85	0.58
1:A:309:SER:HA	1:A:312:GLU:HG3	1.85	0.58
1:B:174:GLY:O	1:B:178:GLY:N	2.35	0.58
1:C:267:ARG:HG2	1:C:267:ARG:NH1	2.18	0.58
1:A:276:LEU:C	1:A:276:LEU:HD13	2.29	0.58
1:F:179:VAL:CG1	1:F:183:SER:HB2	2.33	0.58
1:A:170:ARG:HD2	1:A:184:CYS:O	2.04	0.58
1:C:191:GLU:HG3	1:C:322:LEU:HD21	1.86	0.58
1:E:272:ILE:O	1:E:289:SER:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:GLN:HB2	1:H:108:LEU:CD1	2.33	0.58
1:H:327:LYS:HG3	5:H:1120:HOH:O	2.03	0.58
1:B:246:TYR:CD2	1:B:248:THR:CG2	2.85	0.58
1:G:291:PRO:HB2	1:G:303:VAL:HB	1.85	0.58
1:A:182:LEU:HG	5:C:946:HOH:O	2.03	0.58
1:A:246:TYR:CD1	1:A:248:THR:HG23	2.39	0.58
5:A:822:HOH:O	1:D:304:LYS:HE3	2.03	0.57
1:E:100:GLN:CG	1:E:101:GLU:N	2.20	0.57
1:G:244:LYS:CE	1:H:63:ASP:OD1	2.52	0.57
1:A:317:LYS:O	1:A:321:THR:HG23	2.03	0.57
1:C:51:ASP:OD1	1:C:52:VAL:N	2.38	0.57
1:C:324:GLY:CA	1:C:327:LYS:NZ	2.67	0.57
1:F:246:TYR:CE2	1:F:248:THR:HG21	2.38	0.57
1:G:154:LYS:HE3	1:G:275:MET:CE	2.34	0.57
1:D:180:HIS:CE1	1:D:182:LEU:HD22	2.39	0.57
1:F:328:GLU:C	5:F:896:HOH:O	2.46	0.57
1:A:198:PRO:HG3	1:A:230:HIS:CD2	2.39	0.57
1:A:203:MET:C	1:A:210:LEU:HD13	2.30	0.57
1:B:121:PRO:HD3	1:B:149:ILE:HG21	1.85	0.57
1:C:3:LEU:HD21	1:D:210:LEU:CG	2.20	0.57
1:C:186:GLY:C	1:C:187:TRP:CD1	2.83	0.57
1:D:151:GLY:CA	5:D:1125:HOH:O	2.51	0.57
1:E:98:ARG:HA	1:E:108:LEU:CD1	2.35	0.57
1:A:117:LYS:HA	1:A:149:ILE:HD13	1.87	0.57
1:C:238:TYR:C	1:C:238:TYR:CD2	2.82	0.57
1:D:2:ALA:C	1:D:6:GLN:HE21	2.12	0.57
1:F:283:LYS:N	1:F:283:LYS:CD	2.65	0.57
1:A:279:LEU:HD23	1:A:279:LEU:N	2.18	0.57
1:C:189:LEU:HD11	1:C:291:PRO:HD3	1.87	0.57
1:E:310:GLU:O	1:E:313:ALA:HB3	2.05	0.57
1:F:21:LYS:HB3	1:F:88:SER:HA	1.87	0.57
1:H:204:ASN:ND2	1:H:207:GLY:H	2.03	0.57
1:H:224:GLU:HB2	1:H:226:TRP:HD1	1.70	0.57
1:A:219:THR:HG22	1:A:222:ASP:N	2.20	0.57
1:A:276:LEU:HD13	1:A:276:LEU:O	2.05	0.57
1:C:327:LYS:N	1:C:327:LYS:CE	2.50	0.57
1:D:224:GLU:O	1:D:225:GLN:HB2	2.05	0.57
1:F:187:TRP:HZ3	1:F:271:PRO:HB3	1.69	0.57
1:G:13:LYS:C	1:G:13:LYS:HD3	2.29	0.57
1:B:246:TYR:CE2	1:B:248:THR:HG23	2.38	0.57
1:H:29:ALA:CB	1:H:248:THR:CG2	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLU:CD	1:A:107:ASN:HB3	2.29	0.57
1:A:317:LYS:HD3	1:A:318:SER:N	2.20	0.57
1:B:276:LEU:HD13	1:B:276:LEU:C	2.30	0.57
1:F:191:GLU:CB	1:F:195:SER:OG	2.52	0.57
1:C:211:LYS:NZ	1:C:215:PRO:O	2.37	0.56
1:H:36:ILE:O	1:H:40:MET:HG3	2.05	0.56
1:D:173:MET:HE1	1:D:185:HIS:C	2.30	0.56
1:E:274:THR:O	1:E:287:PHE:HA	2.04	0.56
1:A:234:VAL:C	1:A:236:SER:H	2.12	0.56
1:D:109:VAL:HG12	1:D:329:LEU:HD11	1.86	0.56
1:D:282:ILE:CG2	1:D:283:LYS:N	2.68	0.56
1:D:310:GLU:O	1:D:313:ALA:HB3	2.05	0.56
1:F:53[A]:MET:CE	1:F:56:LYS:NZ	2.66	0.56
1:G:211:LYS:HB2	1:G:217:LEU:HD23	1.87	0.56
1:H:284:GLU:HG2	1:H:316:LYS:HZ1	1.66	0.56
1:H:325:ILE:O	1:H:329:LEU:HD22	2.05	0.56
1:B:164:LEU:HD22	1:B:251:ILE:HB	1.88	0.56
1:G:27:VAL:HG23	1:G:27:VAL:O	2.05	0.56
1:G:154:LYS:CE	1:G:275:MET:HE3	2.35	0.56
1:C:214:HIS:HB2	1:D:3:LEU:HD13	1.87	0.56
1:G:208:VAL:HG22	1:H:7:LEU:CD1	2.35	0.56
1:E:82:TYR:OH	1:E:119:ILE:HG23	2.04	0.56
1:D:220:ASP:C	1:D:222:ASP:H	2.14	0.56
1:E:2:ALA:HB3	1:E:5[B]:ASP:OD2	2.05	0.56
1:B:169:PHE:CD1	1:B:173:MET:CE	2.89	0.56
1:C:28:GLY:HA3	2:C:332:NAI:O5B	2.06	0.56
1:D:75:LYS:HA	1:D:75:LYS:CE	2.35	0.56
2:E:332:NAI:H42N	3:E:333:OXM:O3	2.06	0.56
1:F:27:VAL:HG23	1:F:27:VAL:O	2.05	0.56
1:F:4:LYS:HB3	5:F:954:HOH:O	2.06	0.56
1:H:50:VAL:HB	1:H:79:GLY:O	2.06	0.56
1:H:155:ASN:O	1:H:298:GLY:HA3	2.06	0.56
1:H:169:PHE:CE1	1:H:173:MET:HE1	2.40	0.56
1:F:196:SER:OG	1:F:230:HIS:HE1	1.88	0.55
1:F:330:GLN:CD	1:F:330:GLN:N	2.64	0.55
5:F:877:HOH:O	1:G:19:GLN:HG3	2.05	0.55
1:A:246:TYR:HD1	1:A:248:THR:HG23	1.71	0.55
1:C:124:VAL:HG23	1:C:124:VAL:O	2.06	0.55
1:D:75:LYS:HA	1:D:75:LYS:HE3	1.88	0.55
2:F:332:NAI:H42N	3:F:333:OXM:C1	2.35	0.55
1:H:188:ILE:CG2	1:H:196:SER:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:SER:O	1:B:161:GLY:C	2.50	0.55
1:D:113:VAL:HG21	1:D:329:LEU:HG	1.87	0.55
1:D:216:GLU:O	1:D:222:ASP:CB	2.54	0.55
1:E:316:LYS:HD2	1:E:316:LYS:O	2.06	0.55
1:G:28:GLY:HA3	2:G:332:NAI:O2A	2.06	0.55
1:G:244:LYS:HE2	1:H:63:ASP:OD1	2.05	0.55
1:A:103:GLU:OE1	1:A:104:SER:CA	2.55	0.55
1:D:27:VAL:HG22	1:D:51:ASP:OD2	2.06	0.55
1:G:204:ASN:HA	1:G:210:LEU:HD12	1.85	0.55
1:G:243:LEU:HB3	1:H:55:ASP:O	2.07	0.55
1:H:327:LYS:HD3	5:H:1120:HOH:O	2.06	0.55
1:B:29:ALA:CB	1:B:248:THR:CG2	2.81	0.55
1:C:187:TRP:CD1	1:C:187:TRP:N	2.75	0.55
1:D:248:THR:CB	5:D:559:HOH:O	2.55	0.55
1:D:283:LYS:CE	1:D:316:LYS:HG3	2.37	0.55
1:F:29:ALA:CB	1:F:248:THR:HG22	2.33	0.55
1:A:165:ASP:CG	5:A:373:HOH:O	2.50	0.55
5:B:413:HOH:O	1:C:74:PRO:HB2	2.05	0.55
1:E:62:MET:HE2	1:F:240:VAL:HG22	1.89	0.55
1:D:282:ILE:HG22	1:D:283:LYS:N	2.23	0.55
5:E:373:HOH:O	1:H:74:PRO:HB2	2.05	0.55
1:A:86:ALA:O	1:A:87:ASN:HB2	2.06	0.54
1:H:32:MET:HE1	1:H:64:LEU:HD11	1.88	0.54
1:A:111:ARG:NH1	1:A:111:ARG:CG	2.64	0.54
1:F:163:ASN:HB3	5:F:510:HOH:O	2.05	0.54
1:H:242:LYS:O	1:H:242:LYS:HG3	2.08	0.54
1:A:108:LEU:HD11	1:A:112:ASN:HD21	1.70	0.54
1:A:301:ASP:HB3	1:D:8:ILE:HG22	1.88	0.54
1:B:173:MET:HG2	1:B:184:CYS:HB3	1.89	0.54
1:D:282:ILE:CG2	1:D:283:LYS:H	2.20	0.54
1:H:277:LYS:CD	1:H:283:LYS:O	2.56	0.54
1:E:291:PRO:HB2	1:E:303:VAL:HB	1.88	0.54
1:H:130:CYS:O	1:H:156:ARG:NH1	2.39	0.54
1:A:136:SER:HA	2:A:332:NAI:H1D	1.90	0.54
1:A:233:VAL:O	1:A:236:SER:HB3	2.07	0.54
1:D:241:ILE:HG12	1:D:246:TYR:HA	1.90	0.54
1:H:212:THR:O	1:H:213:LEU:C	2.49	0.54
1:G:109:VAL:HG13	1:G:110:GLN:N	2.22	0.54
1:B:21:LYS:HE3	1:B:46:GLU:CD	2.33	0.54
1:E:331:PHE:N	1:E:331:PHE:CD2	2.76	0.54
1:A:71:LEU:C	5:A:374:HOH:O	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:VAL:HG11	1:B:150:SER:HB2	1.90	0.54
1:E:3:LEU:HA	1:E:6:GLN:HE21	1.72	0.54
1:A:233:VAL:O	1:A:236:SER:CB	2.56	0.54
1:B:316:LYS:O	1:B:316:LYS:HG2	2.07	0.54
1:C:13:LYS:O	1:C:13:LYS:CD	2.56	0.54
1:D:308:THR:CG2	1:D:310:GLU:HB2	2.38	0.54
1:E:53:MET:CE	2:E:332:NAI:O2B	2.56	0.54
1:C:27:VAL:HG23	1:C:27:VAL:O	2.08	0.54
1:F:191:GLU:HB3	1:F:195:SER:OG	2.08	0.54
1:G:120:ILE:O	1:G:124:VAL:HG12	2.05	0.54
1:H:317:LYS:NZ	1:H:317:LYS:CB	2.57	0.54
1:A:203:MET:O	1:A:210:LEU:CD1	2.56	0.53
1:D:25:VAL:HG22	1:D:50[B]:VAL:HG21	1.88	0.53
1:H:189:LEU:N	1:H:189:LEU:HD13	2.21	0.53
1:A:237:ALA:O	1:A:241:ILE:HG13	2.09	0.53
1:D:13:LYS:NZ	1:D:14:GLU:HG2	2.23	0.53
1:E:27:VAL:HG11	1:E:57:LEU:CD1	2.35	0.53
1:E:53:MET:HE3	2:E:332:NAI:O2B	2.08	0.53
1:E:200:TRP:CZ3	1:E:203:MET:HE1	2.43	0.53
1:G:277:LYS:HE3	1:G:285:ASP:OD1	2.08	0.53
1:H:240:VAL:CG1	1:H:247:THR:HG22	2.38	0.53
1:B:154:LYS:HE3	5:B:419:HOH:O	2.08	0.53
1:C:246:TYR:HD2	1:C:248:THR:HG22	1.69	0.53
1:E:19:GLN:O	1:E:89:LYS:HE2	2.08	0.53
1:E:106:LEU:HD21	1:E:328:GLU:HB3	1.90	0.53
1:A:120:ILE:HB	1:A:121:PRO:HD3	1.91	0.53
1:B:235:ASP:O	1:B:239:GLU:HG2	2.08	0.53
1:D:272:ILE:O	1:D:289:SER:HA	2.09	0.53
1:F:18:PRO:HG3	5:F:359:HOH:O	2.07	0.53
1:H:284:GLU:HG3	1:H:316:LYS:HZ2	1.73	0.53
1:E:318:SER:O	1:E:322:LEU:HB2	2.07	0.53
1:B:81:ASP:HB2	5:B:1157:HOH:O	2.08	0.53
1:C:45:ASP:O	1:C:74:PRO:HD2	2.09	0.53
1:E:279:LEU:C	1:E:281:GLY:H	2.16	0.53
1:B:18:PRO:HD2	1:B:18:PRO:O	2.09	0.53
1:E:169:PHE:CD2	1:E:233:VAL:HG21	2.36	0.53
1:A:317:LYS:O	1:A:321:THR:CG2	2.57	0.53
1:C:32:MET:HE1	1:C:64:LEU:HD11	1.91	0.53
1:D:131:LYS:HD3	1:D:131:LYS:N	2.24	0.53
1:A:108:LEU:CD1	1:A:112:ASN:HD21	2.22	0.53
1:A:225:GLN:O	1:A:228:GLN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:MET:CG	1:G:287:PHE:CE2	2.92	0.53
1:B:7:LEU:HD21	1:B:8:ILE:CD1	2.38	0.52
1:B:318:SER:C	1:B:322:LEU:HD23	2.27	0.52
1:C:280:TYR:OH	1:C:303:VAL:O	2.21	0.52
1:G:100:GLN:O	1:G:101:GLU:C	2.48	0.52
1:D:26:GLY:O	1:D:31:GLY:HA3	2.09	0.52
1:E:20:ASN:HB3	5:E:524:HOH:O	2.09	0.52
1:C:327:LYS:HA	5:C:985:HOH:O	2.09	0.52
1:G:231:LYS:HB3	5:G:1008:HOH:O	2.10	0.52
1:H:214:HIS:ND1	1:H:216:GLU:OE2	2.42	0.52
1:A:104:SER:C	1:A:106:LEU:H	2.17	0.52
1:E:143:THR:HG22	1:E:287:PHE:CE1	2.44	0.52
1:E:290:VAL:CG1	1:E:302:VAL:HG13	2.40	0.52
1:C:81:ASP:HB3	5:C:625:HOH:O	2.09	0.52
1:D:29:ALA:C	1:D:248:THR:HG22	2.33	0.52
1:E:296:GLN:NE2	5:E:440:HOH:O	2.31	0.52
1:H:211:LYS:O	1:H:215:PRO:HA	2.09	0.52
1:A:173:MET:HE2	1:A:184:CYS:HB3	1.91	0.52
1:B:246:TYR:CE2	1:B:248:THR:HG21	2.45	0.52
1:E:26:GLY:O	1:E:31:GLY:HA3	2.10	0.52
1:F:318:SER:O	1:F:321:THR:HB	2.10	0.52
1:A:29:ALA:CB	1:A:248:THR:CG2	2.86	0.52
1:C:198:PRO:HG3	1:C:230:HIS:CG	2.45	0.52
1:D:3:LEU:HA	1:D:6:GLN:NE2	2.25	0.52
1:D:10:ASN:HD21	1:D:13:LYS:CG	2.17	0.52
1:G:244:LYS:NZ	1:H:63:ASP:OD1	2.42	0.52
1:H:20:ASN:O	1:H:44:ALA:HA	2.10	0.52
1:A:17:VAL:O	1:A:17:VAL:CG1	2.46	0.52
1:A:264[B]:LYS:CE	5:A:738:HOH:O	2.58	0.52
1:B:223:LYS:HZ3	1:B:224:GLU:HG2	1.75	0.52
1:H:21:LYS:HG3	1:H:46:GLU:HB3	1.91	0.52
1:A:137:ASN:HB2	2:A:332:NAI:O2D	2.10	0.52
1:D:137:ASN:HB2	2:D:332:NAI:O2D	2.10	0.52
1:C:324:GLY:HA2	1:C:327:LYS:HZ1	1.74	0.51
1:D:308:THR:HG21	1:D:310:GLU:HB2	1.92	0.51
1:G:131:LYS:HD3	1:G:131:LYS:N	2.26	0.51
1:C:16:HIS:ND1	1:C:16:HIS:C	2.67	0.51
1:E:173:MET:O	1:E:174:GLY:C	2.53	0.51
1:H:170:ARG:HD2	1:H:184:CYS:O	2.10	0.51
1:H:191:GLU:OE2	1:H:322:LEU:HD13	2.11	0.51
1:B:7:LEU:HD23	1:B:8:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:CD	1:A:285:ASP:OD2	2.56	0.51
1:B:36:ILE:O	1:B:40:MET:HG3	2.10	0.51
1:D:137:ASN:N	2:D:332:NAI:O2D	2.32	0.51
1:E:214:HIS:NE2	1:E:224:GLU:OE1	2.43	0.51
1:E:314:HIS:O	1:E:315:LEU:C	2.52	0.51
1:A:9:HIS:HB2	1:D:304:LYS:HE3	1.91	0.51
1:C:169:PHE:CE2	1:C:229:VAL:HG12	2.45	0.51
1:C:220:ASP:OD1	1:C:227:LYS:HE2	2.10	0.51
1:E:120:ILE:N	1:E:121:PRO:CD	2.74	0.51
1:F:109:VAL:HG23	1:F:110:GLN:N	2.24	0.51
2:G:332:NAI:H42N	3:G:333:OXM:C1	2.40	0.51
1:H:321:THR:O	1:H:322:LEU:C	2.54	0.51
1:C:324:GLY:C	1:C:327:LYS:HZ2	2.17	0.51
1:D:25:VAL:HG22	1:D:50[B]:VAL:CG2	2.41	0.51
1:D:307:LEU:HB2	5:D:347:HOH:O	2.11	0.51
1:E:226:TRP:CE3	1:E:229:VAL:HG21	2.46	0.51
1:F:159:GLY:HA3	1:F:273:SER:HB3	1.92	0.51
1:F:246:TYR:HE2	1:F:248:THR:CG2	2.20	0.51
1:G:6:GLN:HE21	1:H:213:LEU:HG	1.75	0.51
1:G:272:ILE:O	1:G:289:SER:HA	2.11	0.51
1:H:109:VAL:O	1:H:113:VAL:HG23	2.11	0.51
1:F:109:VAL:HG12	1:F:138:PRO:HG2	1.90	0.51
1:F:276:LEU:HD21	1:F:288:LEU:HD11	1.93	0.51
1:F:279:LEU:HD22	1:F:279:LEU:H	1.75	0.51
1:F:283:LYS:HD3	1:F:316:LYS:HE3	1.92	0.51
1:E:268:ARG:HD3	1:G:182:LEU:HD23	1.92	0.51
1:E:279:LEU:C	1:E:281:GLY:N	2.63	0.51
1:B:163:ASN:HB3	5:B:597:HOH:O	2.10	0.51
1:C:246:TYR:CD2	1:C:248:THR:HG22	2.37	0.51
1:D:29:ALA:CB	1:D:248:THR:HG23	2.38	0.51
1:E:279:LEU:O	1:E:280:TYR:HB2	2.10	0.51
1:F:131:LYS:HD3	1:F:131:LYS:N	2.26	0.51
1:F:220:ASP:C	1:F:222:ASP:H	2.19	0.51
1:H:108:LEU:HA	1:H:111:ARG:HB2	1.93	0.51
1:H:200:TRP:CE3	1:H:203:MET:SD	3.04	0.51
1:C:16:HIS:ND1	1:C:17:VAL:N	2.59	0.50
1:C:316:LYS:HA	1:C:319:ALA:HB3	1.93	0.50
1:H:99:GLN:HB2	1:H:108:LEU:HD13	1.91	0.50
1:H:272:ILE:CD1	1:H:294:LEU:HD22	2.41	0.50
1:A:278:GLY:O	1:A:279:LEU:HD23	2.11	0.50
1:C:22:ILE:HG13	1:C:44:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ALA:O	1:C:39:LEU:HD12	2.11	0.50
1:E:94:THR:O	2:E:332:NAI:H52N	2.11	0.50
1:A:211:LYS:O	1:A:215:PRO:CA	2.48	0.50
1:B:330:GLN:HA	1:B:330:GLN:OE1	2.11	0.50
1:E:29:ALA:CB	1:E:248:THR:CG2	2.82	0.50
1:C:69:LEU:HD12	1:D:182:LEU:HD13	1.92	0.50
1:D:97:ALA:H	1:D:112:ASN:ND2	2.08	0.50
1:D:119:ILE:O	1:D:123:VAL:HG13	2.11	0.50
1:E:97:ALA:HB3	1:E:111:ARG:HH21	1.75	0.50
1:B:15:GLU:N	1:B:15:GLU:OE1	2.43	0.50
1:C:165:ASP:OD1	1:C:192:HIS:ND1	2.38	0.50
1:C:317:LYS:NZ	1:C:317:LYS:CB	2.70	0.50
1:C:320:ASP:O	1:C:323:TRP:HB3	2.10	0.50
1:F:179:VAL:CG1	1:F:180:HIS:N	2.74	0.50
1:A:314:HIS:CD2	5:A:578:HOH:O	2.64	0.50
1:E:225:GLN:HG3	1:E:228:GLN:CG	2.31	0.50
1:G:140:ASP:CB	5:G:473:HOH:O	2.48	0.50
1:A:219:THR:CG2	1:A:221:ALA:C	2.85	0.50
1:A:230:HIS:O	1:A:234:VAL:HG13	2.12	0.50
1:D:237:ALA:O	1:D:238:TYR:C	2.54	0.50
1:A:222:ASP:O	1:A:223:LYS:C	2.53	0.50
5:A:822:HOH:O	1:D:304:LYS:CE	2.59	0.50
1:C:324:GLY:C	1:C:327:LYS:HZ1	2.17	0.50
1:D:105:ARG:HD3	1:D:325:ILE:CD1	2.42	0.50
1:D:228:GLN:O	1:D:231:LYS:HB3	2.12	0.50
1:A:108:LEU:O	1:A:109:VAL:C	2.55	0.49
1:A:305:VAL:HG12	1:A:306:THR:N	2.25	0.49
1:B:276:LEU:C	1:B:276:LEU:CD1	2.83	0.49
1:B:301:ASP:HB3	1:C:8:ILE:CG2	2.42	0.49
1:C:26:GLY:O	1:C:31:GLY:HA3	2.12	0.49
1:C:210:LEU:HG	1:D:3:LEU:HD21	1.93	0.49
1:D:151:GLY:HA2	5:D:1125:HOH:O	2.12	0.49
1:D:245:GLY:O	1:D:246:TYR:HB3	2.12	0.49
1:G:214:HIS:CE1	1:G:216:GLU:OE2	2.65	0.49
1:H:105:ARG:O	1:H:108:LEU:HD23	2.12	0.49
1:H:248:THR:HB	5:H:705:HOH:O	2.04	0.49
1:E:14:GLU:O	1:E:14:GLU:CD	2.54	0.49
1:A:264[A]:LYS:HE3	5:A:738:HOH:O	2.11	0.49
1:A:291:PRO:HB2	1:A:303:VAL:HB	1.93	0.49
1:B:120:ILE:O	1:B:124:VAL:HG13	2.12	0.49
1:C:323:TRP:CE3	1:C:323:TRP:CA	2.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ASN:C	1:D:204:ASN:HD22	2.20	0.49
1:G:204:ASN:HD22	1:G:207:GLY:N	2.10	0.49
1:H:97:ALA:N	1:H:112:ASN:OD1	2.42	0.49
1:H:291:PRO:HB2	1:H:303:VAL:HB	1.94	0.49
1:G:214:HIS:HB2	1:H:3:LEU:CD1	2.38	0.49
1:A:314:HIS:C	1:A:317:LYS:HG3	2.37	0.49
1:A:316:LYS:HE2	5:A:942:HOH:O	2.12	0.49
1:H:29:ALA:CB	1:H:248:THR:HG23	2.42	0.49
1:E:267:ARG:NH2	1:G:178:GLY:O	2.41	0.49
1:G:205:VAL:HB	1:H:7:LEU:HD21	1.95	0.49
1:A:180:HIS:ND1	1:A:182:LEU:HB2	2.28	0.49
1:D:29:ALA:O	1:D:248:THR:CG2	2.56	0.49
1:D:112:ASN:O	1:D:113:VAL:C	2.53	0.49
1:E:14:GLU:O	1:E:14:GLU:OE2	2.31	0.49
1:E:163:ASN:ND2	1:E:254:SER:HB2	2.26	0.49
1:F:94:THR:O	2:F:332:NAI:C5D	2.61	0.49
1:A:56:LYS:HE3	5:A:340:HOH:O	2.11	0.49
1:A:317:LYS:C	1:A:317:LYS:CD	2.85	0.49
1:C:3:LEU:HD13	1:D:214:HIS:CB	2.34	0.49
1:C:277:LYS:HE2	1:C:283:LYS:O	2.13	0.49
1:D:105:ARG:O	1:D:106:LEU:C	2.55	0.49
1:E:99:GLN:CB	1:E:111:ARG:HG3	2.38	0.49
1:E:211:LYS:CB	5:E:436:HOH:O	2.60	0.49
1:E:225:GLN:CG	1:E:228:GLN:CG	2.89	0.49
1:H:327:LYS:CG	5:H:1120:HOH:O	2.60	0.49
1:D:244:LYS:HE2	1:D:246:TYR:O	2.13	0.49
1:E:97:ALA:HB3	1:E:111:ARG:NH2	2.28	0.49
1:E:281:GLY:HA2	5:E:541:HOH:O	2.11	0.49
1:H:238:TYR:CD1	1:H:238:TYR:C	2.91	0.49
1:A:143:THR:HG22	1:A:287:PHE:CE1	2.47	0.49
1:A:204:ASN:ND2	5:A:582:HOH:O	2.28	0.49
1:A:296:GLN:HE22	1:D:19:GLN:CG	2.26	0.49
1:D:13:LYS:HZ2	1:D:14:GLU:HG2	1.77	0.49
1:F:109:VAL:HG13	1:F:138:PRO:CG	2.43	0.49
1:G:32:MET:HE2	1:G:60:GLU:HB3	1.95	0.49
1:H:214:HIS:CE1	1:H:216:GLU:HG2	2.48	0.49
1:A:286:VAL:HG13	1:A:322:LEU:HD23	1.95	0.48
1:E:321:THR:O	1:E:325:ILE:HG13	2.12	0.48
1:F:18:PRO:HG2	1:F:87:ASN:CB	2.43	0.48
1:F:300:SER:O	1:F:301:ASP:CG	2.55	0.48
1:A:9:HIS:CD2	1:A:11:LEU:HD23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLU:OE1	1:A:284:GLU:HA	2.13	0.48
1:D:3:LEU:HA	1:D:6:GLN:HE21	1.79	0.48
1:D:117:LYS:HE3	1:D:331:PHE:OXT	2.11	0.48
1:E:105:ARG:CZ	1:E:108:LEU:HD22	2.42	0.48
1:A:265:ASN:OD1	1:A:296:GLN:HG2	2.13	0.48
1:D:129:HIS:ND1	5:D:1040:HOH:O	2.35	0.48
1:E:99:GLN:HB3	1:E:111:ARG:CG	2.41	0.48
1:E:210:LEU:HG	1:F:3:LEU:HD21	1.93	0.48
1:E:214:HIS:HE1	1:E:222:ASP:OD1	1.97	0.48
1:F:200:TRP:HH2	1:F:227:LYS:HA	1.79	0.48
1:F:291:PRO:HB2	1:F:303:VAL:HB	1.94	0.48
1:H:30:VAL:HB	2:H:332:NAI:O2N	2.12	0.48
1:A:214:HIS:CG	1:A:214:HIS:O	2.67	0.48
1:C:143:THR:HG22	1:C:287:PHE:CD1	2.48	0.48
1:F:317:LYS:O	1:F:318:SER:C	2.56	0.48
1:H:219:THR:HG22	1:H:220:ASP:CA	2.37	0.48
1:A:246:TYR:N	1:A:246:TYR:CD2	2.80	0.48
1:E:2:ALA:O	1:E:6:GLN:HG3	2.13	0.48
1:F:286:VAL:O	1:F:286:VAL:HG12	2.09	0.48
1:G:146:ALA:O	1:G:150:SER:HB3	2.13	0.48
1:H:131:LYS:HD2	1:H:131:LYS:N	2.29	0.48
1:B:8:ILE:CG2	1:C:301:ASP:HB3	2.43	0.48
1:D:29:ALA:CB	1:D:248:THR:CG2	2.88	0.48
1:H:179:VAL:HG12	1:H:180:HIS:N	2.28	0.48
1:C:228:GLN:HA	1:C:231:LYS:HB3	1.95	0.48
1:E:239:GLU:HA	1:E:239:GLU:OE2	2.13	0.48
1:F:211:LYS:O	1:F:211:LYS:HG3	2.13	0.48
1:G:211:LYS:N	5:G:483:HOH:O	2.45	0.48
1:A:121:PRO:HD3	1:A:149:ILE:HG21	1.96	0.48
1:A:141:ILE:O	1:A:144:TYR:HB3	2.13	0.48
1:A:313:ALA:O	1:A:317:LYS:HG3	2.14	0.48
1:B:15:GLU:C	1:B:16:HIS:CD2	2.91	0.48
1:B:54:GLU:HG3	1:B:80[B]:LYS:HD2	1.94	0.48
1:B:112:ASN:HD22	1:B:115:ILE:HD12	1.79	0.48
1:D:176:ARG:NH2	1:D:229:VAL:HG23	2.28	0.48
2:F:332:NAI:H3B	5:F:1065:HOH:O	2.12	0.48
2:D:332:NAI:H6N	2:D:332:NAI:C5D	2.44	0.48
1:F:39:LEU:HD11	1:F:64:LEU:HD13	1.96	0.48
1:G:14:GLU:O	1:G:14:GLU:HG3	2.13	0.48
1:G:208:VAL:HG21	1:H:7:LEU:CD1	2.42	0.48
1:G:251:ILE:O	1:G:255:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:169:PHE:CE1	1:H:173:MET:CE	2.97	0.48
1:A:210:LEU:HD12	1:A:210:LEU:H	1.79	0.48
1:C:29:ALA:HB1	1:C:248:THR:CG2	2.43	0.48
1:E:155:ASN:O	1:E:298:GLY:HA3	2.13	0.48
5:E:342:HOH:O	1:H:264:LYS:HD3	2.13	0.48
1:A:1:ALA:O	1:A:2:ALA:O	2.32	0.47
1:A:96:GLY:N	5:A:1095:HOH:O	2.47	0.47
1:C:222:ASP:C	1:C:223:LYS:HD2	2.32	0.47
1:E:14:GLU:OE2	1:E:16:HIS:HB2	2.12	0.47
1:E:82:TYR:CG	1:E:122:ASN:HB3	2.49	0.47
1:A:19:GLN:HG2	1:D:296:GLN:NE2	2.29	0.47
1:A:105:ARG:HG2	1:A:108:LEU:HD23	1.97	0.47
1:C:85:THR:O	1:C:85:THR:HG22	2.14	0.47
1:D:43:LEU:HD23	1:D:264[A]:LYS:HE2	1.95	0.47
1:D:173:MET:HE1	1:D:185:HIS:O	2.14	0.47
1:E:170:ARG:HH21	1:F:69:LEU:HD21	1.79	0.47
1:G:35:ALA:O	1:G:39:LEU:HG	2.14	0.47
1:H:311:GLU:OE2	5:H:361:HOH:O	2.20	0.47
1:A:1:ALA:C	1:A:2:ALA:O	2.56	0.47
1:A:100:GLN:CB	1:A:111:ARG:NH2	2.77	0.47
1:D:124:VAL:O	1:D:124:VAL:HG23	2.15	0.47
1:E:83:SER:C	1:E:85:THR:H	2.21	0.47
1:E:117:LYS:HB2	1:E:117:LYS:HE3	1.58	0.47
1:F:191:GLU:HB2	1:F:195:SER:OG	2.13	0.47
1:B:318:SER:O	1:B:322:LEU:CD2	2.36	0.47
1:C:29:ALA:HB1	1:C:248:THR:HG21	1.96	0.47
1:H:214:HIS:CE1	1:H:216:GLU:CG	2.98	0.47
1:D:32:MET:HE1	1:D:64:LEU:HD11	1.95	0.47
1:B:27:VAL:HG23	1:B:27:VAL:O	2.14	0.47
1:B:137:ASN:ND2	2:B:332:NAI:C2N	2.78	0.47
1:B:317:LYS:HB2	1:B:317:LYS:HE3	1.46	0.47
1:C:18:PRO:HB3	1:C:46:GLU:OE2	2.15	0.47
1:C:198:PRO:HG3	1:C:230:HIS:CD2	2.49	0.47
1:D:29:ALA:C	1:D:248:THR:CG2	2.88	0.47
1:E:99:GLN:HB2	1:E:111:ARG:NH1	2.25	0.47
1:G:17:VAL:O	1:G:17:VAL:HG22	2.15	0.47
1:B:223:LYS:HD3	1:B:224:GLU:HG3	1.97	0.47
1:C:266:LEU:O	1:C:267:ARG:HB2	2.15	0.47
1:C:326:GLN:O	1:C:329:LEU:HB2	2.15	0.47
1:D:109:VAL:CG1	1:D:329:LEU:HD11	2.45	0.47
1:D:155:ASN:O	1:D:298:GLY:HA3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:LYS:HD2	1:E:148:LYS:HA	1.46	0.47
1:E:182:LEU:HD13	1:F:69:LEU:HD12	1.95	0.47
1:E:223:LYS:CD	1:E:223:LYS:O	2.63	0.47
1:F:259:ALA:O	1:F:263:MET:HG2	2.14	0.47
1:F:302:VAL:HG23	1:G:11:LEU:HD11	1.97	0.47
1:H:141:ILE:O	1:H:144:TYR:HB3	2.15	0.47
1:H:173:MET:HE2	1:H:173:MET:HB2	1.79	0.47
1:H:187:TRP:HZ3	1:H:271:PRO:HD3	1.80	0.47
1:H:204:ASN:HD22	1:H:207:GLY:H	1.60	0.47
1:H:330:GLN:O	1:H:331:PHE:HB3	2.14	0.47
1:A:154:LYS:HG2	5:A:936:HOH:O	2.15	0.47
1:C:204:ASN:HD22	1:C:207:GLY:H	1.62	0.47
1:D:12:LEU:O	1:D:13:LYS:HG2	2.15	0.47
1:G:277:LYS:O	1:G:277:LYS:HG3	2.14	0.47
1:H:173:MET:SD	1:H:184:CYS:HB3	2.55	0.47
1:A:117:LYS:HG2	1:A:149:ILE:HD11	1.97	0.47
1:B:18:PRO:O	1:B:18:PRO:CD	2.61	0.47
1:C:213:LEU:HD12	1:C:213:LEU:HA	1.71	0.47
1:E:12:LEU:HD11	1:H:297:ASN:HB3	1.95	0.47
1:E:81:ASP:OD2	1:E:81:ASP:C	2.57	0.47
1:F:18:PRO:CG	1:F:87:ASN:HB2	2.45	0.47
1:G:219:THR:HG22	1:G:221:ALA:H	1.78	0.47
1:B:130:CYS:O	1:B:156:ARG:HD2	2.15	0.47
1:C:188:ILE:O	1:C:189:LEU:HD12	2.15	0.47
1:D:119:ILE:HD11	2:D:332:NAI:C6A	2.45	0.47
1:D:196:SER:OG	1:D:230:HIS:CE1	2.67	0.47
1:E:58:LYS:O	1:E:62:MET:HG3	2.15	0.47
1:E:231:LYS:HD2	1:E:231:LYS:HA	1.37	0.47
1:G:271:PRO:O	1:G:271:PRO:HG2	2.15	0.47
1:G:315:LEU:HD12	1:G:315:LEU:HA	1.62	0.47
1:B:284:GLU:HA	1:B:284:GLU:OE1	2.15	0.46
1:E:3:LEU:HA	1:E:6:GLN:HG3	1.97	0.46
1:E:46:GLU:CG	1:E:75:LYS:HD3	2.45	0.46
1:F:153:PRO:HB2	1:F:155:ASN:OD1	2.14	0.46
1:B:290:VAL:HG13	1:B:302:VAL:HG13	1.97	0.46
1:E:191:GLU:O	1:E:192:HIS:C	2.57	0.46
1:E:324:GLY:O	1:E:327:LYS:HG2	2.15	0.46
1:C:310:GLU:O	1:C:313:ALA:HB3	2.14	0.46
1:D:82:TYR:OH	1:D:119:ILE:HG12	2.16	0.46
1:D:105:ARG:NH1	5:D:1144:HOH:O	2.47	0.46
1:E:36:ILE:O	1:E:40:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:ILE:C	1:E:189:LEU:HD13	2.40	0.46
1:B:143:THR:HG22	1:B:287:PHE:CE1	2.50	0.46
1:D:283:LYS:NZ	1:D:316:LYS:HE2	2.29	0.46
4:E:334:ACT:CH3	5:E:532:HOH:O	2.63	0.46
1:G:154:LYS:HE3	1:G:275:MET:HE3	1.96	0.46
1:G:240:VAL:CG1	1:G:247:THR:HG22	2.45	0.46
1:H:188:ILE:HG22	1:H:196:SER:HB2	1.96	0.46
1:H:205:VAL:O	1:H:208:VAL:HG13	2.16	0.46
1:B:211:LYS:O	1:B:211:LYS:HG2	2.14	0.46
1:C:211:LYS:CB	5:C:638:HOH:O	2.63	0.46
1:C:276:LEU:CD2	1:C:288:LEU:HD11	2.45	0.46
1:C:121:PRO:HA	5:C:380:HOH:O	2.15	0.46
1:F:19:GLN:N	5:F:354:HOH:O	2.32	0.46
1:G:72:ARG:NE	5:G:358:HOH:O	2.41	0.46
1:C:143:THR:HG22	1:C:287:PHE:CE1	2.51	0.46
1:D:216:GLU:O	1:D:222:ASP:CG	2.59	0.46
1:E:73:THR:OG1	5:E:906:HOH:O	2.21	0.46
1:F:27:VAL:O	1:F:56:LYS:HE3	2.16	0.46
1:H:189:LEU:HD12	1:H:189:LEU:HA	1.57	0.46
1:G:180:HIS:ND1	1:G:182:LEU:HB2	2.31	0.46
1:H:152:PHE:N	5:H:347:HOH:O	2.48	0.46
1:A:166:SER:O	1:A:170:ARG:HG3	2.15	0.46
1:A:296:GLN:NE2	1:D:19:GLN:CG	2.79	0.46
1:C:198:PRO:HD3	1:C:230:HIS:NE2	2.31	0.46
1:E:110:GLN:HA	1:E:110:GLN:NE2	2.31	0.46
1:E:219:THR:HG21	1:E:221:ALA:HB3	1.97	0.46
1:G:189:LEU:HD11	1:G:291:PRO:HD3	1.97	0.46
1:H:131:LYS:HD2	1:H:131:LYS:H	1.80	0.46
1:H:194:ASP:HA	1:H:234:VAL:HG13	1.98	0.46
1:A:105:ARG:NH1	1:A:105:ARG:CG	2.71	0.46
1:B:26:GLY:O	1:B:31:GLY:HA3	2.15	0.46
1:C:87:ASN:HA	4:C:334:ACT:OXT	2.16	0.46
1:C:228:GLN:HA	1:C:231:LYS:CB	2.46	0.46
1:E:219:THR:HG23	1:E:220:ASP:N	2.31	0.46
1:F:266:LEU:O	1:H:180:HIS:HB2	2.15	0.46
1:G:143:THR:CG2	1:G:157:VAL:HG12	2.46	0.46
1:A:108:LEU:HD12	1:A:108:LEU:O	2.16	0.45
1:B:169:PHE:CE1	1:B:173:MET:HE1	2.49	0.45
1:C:85:THR:O	1:C:85:THR:HG23	2.15	0.45
1:C:214:HIS:CB	1:D:3:LEU:HD13	2.46	0.45
1:E:189:LEU:HD12	1:E:189:LEU:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TRP:CE3	1:A:203:MET:SD	3.09	0.45
1:A:323:TRP:O	1:A:327:LYS:HB3	2.16	0.45
1:B:169:PHE:CD1	1:B:173:MET:HE2	2.51	0.45
1:D:100:GLN:O	1:D:101:GLU:C	2.58	0.45
1:E:28:GLY:HA3	2:E:332:NAI:O5B	2.16	0.45
2:E:332:NAI:N1A	5:E:568:HOH:O	2.36	0.45
1:C:139:VAL:O	1:C:139:VAL:HG22	2.16	0.45
1:D:236:SER:O	1:D:240:VAL:HG23	2.17	0.45
1:F:169:PHE:HD2	1:F:233:VAL:HG21	1.81	0.45
1:G:180:HIS:CE1	1:G:182:LEU:HD22	2.52	0.45
1:H:27:VAL:HG23	1:H:56:LYS:HD3	1.97	0.45
1:A:169:PHE:CD2	1:A:188:ILE:HD11	2.51	0.45
1:A:290:VAL:CG1	1:A:302:VAL:HG13	2.47	0.45
1:D:283:LYS:H	1:D:283:LYS:HG2	1.37	0.45
1:E:46:GLU:HG3	1:E:75:LYS:HD3	1.98	0.45
1:E:137:ASN:HA	1:E:138:PRO:C	2.41	0.45
1:E:174:GLY:C	5:E:992:HOH:O	2.60	0.45
1:G:205:VAL:O	1:G:206:ALA:C	2.59	0.45
1:G:211:LYS:O	1:G:211:LYS:HG3	2.16	0.45
1:C:17:VAL:HA	1:C:18:PRO:HD3	1.80	0.45
1:D:143:THR:HG22	1:D:287:PHE:CE1	2.51	0.45
1:A:301:ASP:HB3	1:D:8:ILE:CG2	2.46	0.45
1:B:107:ASN:HD21	2:F:332:NAI:H2B	1.82	0.45
1:E:228:GLN:OE1	1:E:228:GLN:HA	2.17	0.45
1:F:173:MET:CE	1:F:184:CYS:HB3	2.47	0.45
1:A:2:ALA:CA	1:B:224:GLU:OE2	2.64	0.45
1:A:296:GLN:NE2	1:D:19:GLN:HG3	2.31	0.45
1:B:154:LYS:HD2	1:B:275:MET:HB3	1.99	0.45
1:C:81:ASP:O	1:C:84:VAL:HG13	2.17	0.45
1:F:165:ASP:OD1	1:F:165:ASP:N	2.47	0.45
1:F:192:HIS:O	1:F:192:HIS:CG	2.69	0.45
1:A:214:HIS:NE2	1:A:222:ASP:OD1	2.49	0.45
1:E:180:HIS:CE1	1:E:182:LEU:HD22	2.50	0.45
1:G:217:LEU:HD12	1:G:226:TRP:CB	2.46	0.45
1:H:117:LYS:O	1:H:121:PRO:HG2	2.17	0.45
1:H:235:ASP:O	1:H:236:SER:C	2.56	0.45
1:H:327:LYS:NZ	1:H:327:LYS:HB2	2.21	0.45
1:G:140:ASP:OD2	1:G:191:GLU:HA	2.17	0.45
1:H:124:VAL:O	1:H:124:VAL:HG23	2.16	0.45
1:A:204:ASN:HA	1:A:210:LEU:HD12	1.90	0.45
1:A:301:ASP:OD2	1:D:10:ASN:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:GLN:O	1:B:68:SER:OG	2.35	0.45
1:C:284:GLU:CD	1:C:284:GLU:H	2.25	0.45
1:C:320:ASP:HA	1:C:323:TRP:HB2	1.99	0.45
1:D:19:GLN:O	1:D:89:LYS:HD2	2.17	0.45
1:E:219:THR:CG2	1:E:221:ALA:HB3	2.47	0.45
1:E:311:GLU:C	1:E:313:ALA:N	2.73	0.45
1:C:51:ASP:HA	2:C:332:NAI:H2A	1.99	0.44
1:D:10:ASN:ND2	1:D:13:LYS:HG3	2.21	0.44
1:D:204:ASN:HD22	1:D:205:VAL:N	2.15	0.44
1:F:109:VAL:O	1:F:113:VAL:HG23	2.17	0.44
1:F:204:ASN:HD22	1:F:207:GLY:H	1.65	0.44
1:G:19:GLN:O	1:G:89:LYS:CE	2.65	0.44
1:B:29:ALA:HB1	1:B:248:THR:HG22	1.92	0.44
1:E:251:ILE:HD12	1:E:251:ILE:O	2.17	0.44
1:A:305:VAL:CG1	1:A:306:THR:N	2.80	0.44
1:B:107:ASN:ND2	5:B:393:HOH:O	2.50	0.44
1:B:261:SER:HA	1:B:266:LEU:HB2	1.99	0.44
1:B:290:VAL:CG1	1:B:302:VAL:HG13	2.48	0.44
1:C:123:VAL:HG11	1:C:132:LEU:HD21	2.00	0.44
1:D:2:ALA:HB3	1:D:5:ASP:OD1	2.17	0.44
1:D:152:PHE:HA	1:D:153:PRO:HD3	1.81	0.44
1:E:8:ILE:HG22	1:E:9:HIS:N	2.31	0.44
1:F:105:ARG:NH2	3:F:333:OXM:O2	2.50	0.44
1:F:179:VAL:HG11	1:F:183:SER:HB2	1.99	0.44
1:F:226:TRP:C	1:F:228:GLN:N	2.75	0.44
1:G:267:ARG:HA	1:G:294:LEU:O	2.17	0.44
1:H:228:GLN:O	1:H:232:GLN:N	2.49	0.44
1:E:107:ASN:OD1	1:E:107:ASN:O	2.34	0.44
1:E:153:PRO:HG2	5:E:1192:HOH:O	2.16	0.44
1:F:8:ILE:HG23	1:G:301:ASP:HB3	1.99	0.44
1:F:210:LEU:N	1:F:210:LEU:CD1	2.80	0.44
1:H:29:ALA:C	1:H:248:THR:CG2	2.89	0.44
1:A:219:THR:HG22	1:A:221:ALA:N	2.31	0.44
1:B:308:THR:O	1:B:312:GLU:HG2	2.18	0.44
1:D:50[A]:VAL:HG12	1:D:51:ASP:N	2.33	0.44
1:D:100:GLN:O	1:D:102:GLY:N	2.51	0.44
1:F:192:HIS:O	1:F:192:HIS:HD2	1.98	0.44
1:G:19:GLN:O	1:G:89:LYS:NZ	2.51	0.44
1:H:217:LEU:HD12	1:H:226:TRP:CG	2.53	0.44
1:H:283:LYS:HE3	1:H:283:LYS:HB2	1.43	0.44
1:A:32:MET:HE1	1:A:64:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LYS:HB3	1:A:117:LYS:HE2	1.70	0.44
1:C:223:LYS:HE2	1:C:223:LYS:CA	2.46	0.44
1:D:257:ASP:HB2	5:D:427:HOH:O	2.16	0.44
1:E:170:ARG:HD3	5:E:361:HOH:O	2.17	0.44
1:F:3:LEU:HD12	1:F:3:LEU:O	2.17	0.44
1:A:45:ASP:OD2	5:A:384:HOH:O	2.21	0.44
1:B:170:ARG:HA	1:B:173:MET:HE3	1.99	0.44
1:D:13:LYS:O	1:D:15:GLU:OE2	2.36	0.44
1:H:259:ALA:O	1:H:263:MET:HG2	2.17	0.44
1:A:58:LYS:O	1:A:62:MET:HG3	2.18	0.44
1:B:154:LYS:HD2	1:B:275:MET:HE3	2.00	0.44
1:B:258:LEU:HD23	1:B:258:LEU:HA	1.77	0.44
1:F:18:PRO:CA	5:F:354:HOH:O	2.63	0.44
1:B:123:VAL:HG21	1:B:132:LEU:HD21	1.99	0.44
1:E:223:LYS:HE2	5:E:540:HOH:O	2.17	0.44
1:F:61:MET:O	1:F:65:GLN:HG3	2.18	0.44
1:H:267:ARG:HA	1:H:294:LEU:O	2.18	0.44
1:A:105:ARG:HH11	1:A:108:LEU:HD23	1.80	0.43
1:A:107:ASN:C	1:A:107:ASN:OD1	2.60	0.43
1:C:283:LYS:HA	1:C:283:LYS:CE	2.29	0.43
1:D:198:PRO:HD3	1:D:230:HIS:CE1	2.53	0.43
1:E:240:VAL:CG2	1:F:62:MET:HE2	2.48	0.43
1:G:101:GLU:N	5:G:471:HOH:O	2.38	0.43
1:G:317:LYS:O	1:G:320:ASP:HB2	2.18	0.43
1:H:133:LEU:HA	1:H:158:ILE:O	2.17	0.43
1:A:219:THR:HG22	1:A:221:ALA:C	2.43	0.43
1:C:267:ARG:HH11	1:C:267:ARG:CG	2.30	0.43
1:E:8:ILE:HG23	1:E:9:HIS:H	1.83	0.43
1:E:305:VAL:HA	1:G:208:VAL:HG11	1.99	0.43
1:F:61:MET:HE1	5:F:1146:HOH:O	2.17	0.43
1:F:187:TRP:CE3	1:F:271:PRO:HB3	2.53	0.43
1:G:204:ASN:ND2	1:G:207:GLY:H	2.11	0.43
1:G:276:LEU:HG	1:G:288:LEU:HD12	2.00	0.43
1:A:19:GLN:CG	1:D:296:GLN:NE2	2.81	0.43
1:A:112:ASN:O	1:A:113:VAL:C	2.60	0.43
1:A:155:ASN:O	1:A:298:GLY:HA3	2.19	0.43
1:B:198:PRO:HG2	1:B:198:PRO:O	2.18	0.43
1:D:81:ASP:HB3	5:D:784:HOH:O	2.17	0.43
1:E:219:THR:CG2	1:E:220:ASP:N	2.81	0.43
1:F:109:VAL:CG1	1:F:138:PRO:CG	2.90	0.43
1:G:13:LYS:HD3	1:G:14:GLU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:O	1:A:41:LYS:HG3	2.18	0.43
1:B:310:GLU:H	1:B:310:GLU:HG3	1.51	0.43
1:C:30:VAL:HG22	1:C:251:ILE:HG21	2.01	0.43
1:C:211:LYS:HB3	5:C:638:HOH:O	2.18	0.43
1:D:227:LYS:HE2	5:D:869:HOH:O	2.17	0.43
1:D:307:LEU:CB	5:D:347:HOH:O	2.66	0.43
1:E:311:GLU:C	1:E:313:ALA:H	2.26	0.43
1:G:29:ALA:C	1:G:248:THR:CG2	2.90	0.43
1:B:83:SER:C	1:B:85:THR:H	2.26	0.43
1:C:277:LYS:HD2	1:C:283:LYS:NZ	2.33	0.43
1:D:120:ILE:O	1:D:124:VAL:HG13	2.18	0.43
1:E:180:HIS:HB2	1:G:266:LEU:O	2.19	0.43
1:F:300:SER:OG	1:F:301:ASP:OD1	2.27	0.43
1:G:82:TYR:CG	1:G:122:ASN:HB3	2.53	0.43
1:C:51:ASP:HA	2:C:332:NAI:C2A	2.48	0.43
1:C:155:ASN:ND2	1:C:156:ARG:HG3	2.34	0.43
1:D:36:ILE:HD12	1:D:36:ILE:HA	1.85	0.43
1:E:99:GLN:HB2	1:E:111:ARG:HD3	2.00	0.43
1:F:326:GLN:CB	1:F:329:LEU:HD22	2.45	0.43
1:G:220:ASP:HB2	5:G:693:HOH:O	2.17	0.43
1:A:211:LYS:HD2	1:A:217:LEU:HB3	2.01	0.43
1:E:4:LYS:HG3	1:F:177:LEU:HD12	2.00	0.43
1:G:204:ASN:N	1:G:210:LEU:HD13	2.34	0.43
1:H:106:LEU:HD21	1:H:328:GLU:OE1	2.17	0.43
1:A:264[B]:LYS:NZ	5:A:738:HOH:O	2.48	0.43
1:C:21:LYS:HB3	1:C:88:SER:HA	2.00	0.43
1:C:130:CYS:O	1:C:156:ARG:NH1	2.49	0.43
1:F:105:ARG:HH21	3:F:333:OXM:C1	2.31	0.43
1:G:113:VAL:HG22	1:G:145:VAL:HG21	2.00	0.43
1:G:324:GLY:CA	1:G:327:LYS:HD2	2.49	0.43
1:H:216:GLU:O	1:H:222:ASP:HB2	2.18	0.43
1:A:121:PRO:HD3	1:A:149:ILE:CG2	2.48	0.43
1:A:211:LYS:NZ	1:A:217:LEU:O	2.49	0.43
1:D:118:PHE:HD2	2:D:332:NAI:H62A	1.67	0.43
1:E:30:VAL:HB	2:E:332:NAI:H51N	2.01	0.43
1:F:216:GLU:HG2	1:F:221:ALA:O	2.18	0.43
1:B:180:HIS:ND1	1:B:182:LEU:HB2	2.33	0.43
1:B:330:GLN:OE1	1:B:330:GLN:CA	2.67	0.43
1:C:187:TRP:CE2	5:C:982:HOH:O	2.71	0.43
1:C:220:ASP:OD1	1:C:227:LYS:CE	2.67	0.43
1:C:283:LYS:CA	1:C:283:LYS:CE	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:VAL:O	1:E:149:ILE:HG13	2.19	0.43
1:E:160:SER:O	1:E:161:GLY:C	2.62	0.43
1:F:276:LEU:C	1:F:276:LEU:HD13	2.44	0.43
1:B:246:TYR:HE2	1:B:248:THR:HG21	1.84	0.42
1:C:63:ASP:O	1:D:250:ALA:HB2	2.19	0.42
1:E:276:LEU:HD21	1:E:288:LEU:HB2	2.00	0.42
1:F:75:LYS:HA	1:F:75:LYS:HD3	1.90	0.42
1:G:231:LYS:O	1:G:234:VAL:HG22	2.19	0.42
1:A:148:LYS:HA	1:A:148:LYS:HD2	1.84	0.42
1:A:208:VAL:O	1:A:208:VAL:CG2	2.68	0.42
1:C:323:TRP:O	1:C:327:LYS:NZ	2.49	0.42
1:G:189:LEU:HD22	1:G:199:VAL:HG21	2.01	0.42
1:G:242:LYS:HE2	1:G:242:LYS:HB2	1.44	0.42
1:A:314:HIS:HB3	5:A:753:HOH:O	2.19	0.42
1:C:22:ILE:HD13	1:C:90:LEU:HD23	2.01	0.42
1:D:204:ASN:HB3	5:D:973:HOH:O	2.19	0.42
1:D:220:ASP:O	1:D:222:ASP:N	2.51	0.42
1:F:1:ALA:O	1:F:2:ALA:C	2.62	0.42
1:F:166:SER:O	1:F:170:ARG:HG3	2.19	0.42
1:F:239:GLU:O	1:F:243:LEU:HD22	2.20	0.42
1:H:315:LEU:HD12	1:H:315:LEU:HA	1.85	0.42
1:A:41:LYS:HB3	1:A:41:LYS:HE3	1.78	0.42
1:D:75:LYS:HE3	1:D:75:LYS:CA	2.46	0.42
1:E:105:ARG:O	1:E:109:VAL:CG2	2.66	0.42
1:F:120:ILE:HD13	1:F:120:ILE:HA	1.94	0.42
1:F:316:LYS:HD2	1:F:316:LYS:O	2.18	0.42
1:G:121:PRO:HD3	1:G:149:ILE:HG21	2.02	0.42
1:G:143:THR:HG22	1:G:157:VAL:HG12	2.01	0.42
1:A:264[B]:LYS:HE2	5:A:738:HOH:O	2.19	0.42
1:B:55:ASP:HB2	5:B:949:HOH:O	2.19	0.42
1:C:43:LEU:N	5:C:358:HOH:O	2.52	0.42
1:E:120:ILE:N	1:E:121:PRO:HD2	2.34	0.42
1:G:112:ASN:HA	1:G:115:ILE:HB	2.02	0.42
1:G:123:VAL:C	1:G:125:LYS:H	2.28	0.42
1:H:242:LYS:O	1:H:242:LYS:HG2	2.18	0.42
1:H:331:PHE:CD1	1:H:331:PHE:OXT	2.73	0.42
1:B:39:LEU:O	5:B:342:HOH:O	2.21	0.42
1:E:179:VAL:HG12	1:E:180:HIS:O	2.20	0.42
1:G:75:LYS:HE3	1:G:77:VAL:HG13	2.00	0.42
1:H:110:GLN:O	1:H:113:VAL:HB	2.19	0.42
1:A:200:TRP:CE2	1:A:218:GLY:HA3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:SER:O	1:B:69:LEU:C	2.62	0.42
1:C:117:LYS:HB3	1:C:117:LYS:HE3	1.82	0.42
1:D:282:ILE:HD13	1:D:282:ILE:HA	1.72	0.42
1:E:330:GLN:HE21	1:E:330:GLN:HB3	1.65	0.42
1:F:54:GLU:HG3	1:F:80:LYS:HD2	2.00	0.42
1:F:283:LYS:CD	1:F:283:LYS:H	2.33	0.42
1:B:17:VAL:CG2	1:B:18:PRO:CD	2.98	0.42
1:B:326:GLN:O	1:B:327:LYS:C	2.61	0.42
1:E:61:MET:HE2	1:E:61:MET:HB3	1.85	0.42
1:E:258:LEU:O	1:E:259:ALA:C	2.62	0.42
1:G:231:LYS:HG2	5:G:1008:HOH:O	2.19	0.42
1:H:137:ASN:HA	1:H:139:VAL:N	2.34	0.42
1:H:220:ASP:C	1:H:222:ASP:H	2.28	0.42
1:A:122:ASN:N	1:A:122:ASN:HD22	2.17	0.42
1:B:98:ARG:HB3	2:B:332:NAI:H3D	2.01	0.42
1:C:216:GLU:CG	1:C:222:ASP:HB2	2.50	0.42
1:C:233:VAL:O	1:C:236:SER:HB2	2.20	0.42
1:F:111:ARG:N	5:F:362:HOH:O	2.28	0.42
1:G:276:LEU:HD21	1:G:282:ILE:HD12	2.02	0.42
1:H:120:ILE:N	1:H:121:PRO:CD	2.83	0.42
1:A:9:HIS:CD2	1:A:11:LEU:CD2	3.03	0.42
1:C:314:HIS:O	1:C:315:LEU:C	2.63	0.42
1:E:27:VAL:O	1:E:27:VAL:HG23	2.18	0.42
1:E:170:ARG:HH21	1:F:69:LEU:CD1	2.31	0.42
1:F:237:ALA:O	1:F:241:ILE:CG1	2.66	0.42
1:H:276:LEU:HD13	1:H:276:LEU:O	2.20	0.42
1:H:323:TRP:HA	1:H:326:GLN:HB2	2.02	0.42
1:C:113:VAL:HG12	1:C:114:ASN:N	2.35	0.41
1:D:40:MET:HE2	1:D:40:MET:HB3	1.97	0.41
1:D:291:PRO:HB2	1:D:303:VAL:HB	2.02	0.41
1:E:223:LYS:O	1:E:223:LYS:HD3	2.20	0.41
1:F:206:ALA:HA	1:H:187:TRP:CZ2	2.55	0.41
1:H:106:LEU:HD12	1:H:106:LEU:HA	1.90	0.41
1:A:103:GLU:OE1	1:A:104:SER:N	2.52	0.41
1:A:234:VAL:C	1:A:236:SER:N	2.76	0.41
1:B:41:LYS:HE3	1:B:41:LYS:HB3	1.77	0.41
1:E:109:VAL:O	1:E:113:VAL:HG23	2.20	0.41
1:F:200:TRP:CE2	1:F:218:GLY:HA2	2.55	0.41
1:C:216:GLU:OE2	1:C:223:LYS:HD3	2.21	0.41
1:F:204:ASN:HB2	1:F:208:VAL:O	2.20	0.41
1:H:304:LYS:HE2	1:H:304:LYS:HB2	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:C	1:A:108:LEU:CD1	2.89	0.41
1:E:286:VAL:HG13	1:E:322:LEU:HD23	2.00	0.41
1:H:111:ARG:O	1:H:115:ILE:HG13	2.21	0.41
1:H:180:HIS:ND1	1:H:182:LEU:HB2	2.36	0.41
1:B:97:ALA:H	1:B:112:ASN:ND2	1.96	0.41
1:B:191:GLU:CD	1:B:322:LEU:HD21	2.46	0.41
1:C:240:VAL:CG2	1:D:62:MET:HE2	2.51	0.41
1:C:291:PRO:HB2	1:C:303:VAL:HB	2.01	0.41
1:D:276:LEU:HD12	1:D:276:LEU:H	1.86	0.41
1:H:98:ARG:CD	5:H:1171:HOH:O	2.67	0.41
1:A:210:LEU:CD1	1:A:210:LEU:N	2.83	0.41
1:A:219:THR:HB	1:A:222:ASP:HB2	2.03	0.41
1:A:219:THR:HG21	1:A:221:ALA:C	2.44	0.41
1:C:276:LEU:HD21	1:C:288:LEU:HD11	2.03	0.41
1:F:121:PRO:HG3	1:F:149:ILE:CG2	2.51	0.41
1:G:238:TYR:CD2	1:G:238:TYR:N	2.89	0.41
1:G:244:LYS:HE3	1:G:246:TYR:O	2.20	0.41
1:H:245:GLY:O	1:H:246:TYR:HB3	2.21	0.41
1:A:219:THR:HG23	1:A:221:ALA:N	2.36	0.41
1:D:168:ARG:HD2	5:D:370:HOH:O	2.20	0.41
1:E:290:VAL:HG11	1:E:302:VAL:CG1	2.50	0.41
1:G:20:ASN:HA	1:G:89:LYS:HD3	2.02	0.41
1:G:250:ALA:HB2	1:H:63:ASP:O	2.21	0.41
1:G:323:TRP:O	1:G:327:LYS:CG	2.59	0.41
1:H:276:LEU:C	1:H:276:LEU:CD1	2.94	0.41
1:A:228:GLN:O	1:A:229:VAL:C	2.64	0.41
1:C:146:ALA:O	1:C:150:SER:HB3	2.21	0.41
1:C:267:ARG:HB2	5:C:339:HOH:O	2.20	0.41
1:D:230:HIS:O	1:D:234:VAL:HG12	2.19	0.41
1:E:211:LYS:N	5:E:436:HOH:O	2.46	0.41
1:H:248:THR:CG2	5:H:705:HOH:O	2.57	0.41
1:A:191:GLU:HG3	1:A:318:SER:OG	2.20	0.41
1:A:208:VAL:HG11	1:C:305:VAL:HA	2.02	0.41
1:A:246:TYR:CD1	1:A:248:THR:CG2	3.04	0.41
1:A:290:VAL:HG12	1:A:302:VAL:HG13	2.03	0.41
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.92	0.41
1:C:2:ALA:CA	1:D:224:GLU:OE1	2.67	0.41
1:C:32:MET:HB3	1:D:249:TRP:CZ2	2.56	0.41
1:C:284:GLU:N	1:C:284:GLU:CD	2.79	0.41
1:D:135:VAL:O	1:D:135:VAL:HG12	2.21	0.41
1:D:222:ASP:OD1	1:D:224:GLU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:NAI:H52A	5:D:567:HOH:O	2.21	0.41
1:E:131:LYS:NZ	5:E:668:HOH:O	2.44	0.41
1:E:170:ARG:HH21	1:F:69:LEU:HD11	1.79	0.41
1:E:214:HIS:HB2	1:F:3:LEU:HD13	2.02	0.41
1:F:318:SER:O	1:F:319:ALA:C	2.64	0.41
1:G:46:GLU:OE1	1:G:75:LYS:HG2	2.21	0.41
1:G:55:ASP:O	1:G:56:LYS:C	2.64	0.41
1:G:179:VAL:HG12	1:G:180:HIS:O	2.21	0.41
1:G:189:LEU:O	1:G:197:VAL:N	2.35	0.41
1:A:131:LYS:HB2	1:A:131:LYS:HE3	1.31	0.41
1:A:222:ASP:OD2	1:A:224:GLU:O	2.38	0.41
1:B:169:PHE:HE1	1:B:173:MET:CE	2.30	0.41
1:C:188:ILE:HG22	1:C:196:SER:HB2	2.03	0.41
1:E:300:SER:C	1:E:301:ASP:OD1	2.64	0.41
1:A:119:ILE:HD13	1:A:119:ILE:HG21	1.69	0.40
1:A:189:LEU:HA	1:A:189:LEU:HD12	1.78	0.40
1:B:13:LYS:O	1:B:15:GLU:OE1	2.39	0.40
1:B:173:MET:SD	1:B:184:CYS:HB3	2.61	0.40
1:C:50:VAL:HG23	1:C:51:ASP:N	2.35	0.40
1:C:191:GLU:O	1:C:196:SER:HB3	2.21	0.40
1:D:194:ASP:OD2	1:D:194:ASP:N	2.44	0.40
1:D:220:ASP:C	1:D:222:ASP:N	2.77	0.40
1:E:3:LEU:O	1:E:4:LYS:C	2.64	0.40
1:E:89:LYS:HG2	5:E:351:HOH:O	2.20	0.40
1:F:86:ALA:O	1:F:87:ASN:HB2	2.21	0.40
1:F:173:MET:HE2	1:F:184:CYS:HB3	2.02	0.40
1:G:169:PHE:CE1	1:G:173:MET:HE2	2.56	0.40
1:G:177:LEU:N	1:G:177:LEU:HD13	2.36	0.40
1:H:95:ALA:O	1:H:136:SER:OG	2.30	0.40
1:A:100:GLN:HG3	1:A:111:ARG:NH2	2.36	0.40
1:B:246:TYR:HE2	1:B:248:THR:CG2	2.31	0.40
1:C:160:SER:O	1:C:161:GLY:C	2.64	0.40
1:C:216:GLU:HG3	1:C:222:ASP:HA	2.03	0.40
1:C:247:THR:C	1:C:248:THR:CG2	2.94	0.40
2:C:332:NAI:H42N	3:C:333:OXM:C1	2.51	0.40
1:D:304:LYS:H	1:D:304:LYS:HG2	1.66	0.40
1:F:17:VAL:HA	1:F:18:PRO:HD2	1.80	0.40
1:F:204:ASN:ND2	1:F:207:GLY:HA2	2.37	0.40
1:H:277:LYS:HE3	1:H:285:ASP:CG	2.46	0.40
1:D:28:GLY:O	1:D:29:ALA:C	2.64	0.40
1:G:208:VAL:HG21	1:H:7:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:PRO:CG	1:H:46:GLU:OE1	2.69	0.40
1:H:27:VAL:O	1:H:56:LYS:HE3	2.22	0.40
1:H:272:ILE:HD13	1:H:294:LEU:HD22	2.03	0.40
1:H:308:THR:HG22	1:H:310:GLU:CG	2.31	0.40
1:A:104:SER:C	1:A:106:LEU:N	2.79	0.40
1:C:205:VAL:HB	1:D:7:LEU:HD21	2.03	0.40
1:E:53:MET:HG3	2:E:332:NAI:O2B	2.21	0.40
1:E:181:ALA:O	1:E:182:LEU:C	2.65	0.40
1:E:316:LYS:HD3	1:E:316:LYS:HA	1.94	0.40
5:E:794:HOH:O	1:F:53[B]:MET:CE	2.52	0.40
1:H:219:THR:CG2	1:H:221:ALA:N	2.71	0.40
1:A:127:SER:HB3	1:A:130:CYS:HB3	2.04	0.40
1:B:105:ARG:O	1:B:138:PRO:HD3	2.22	0.40
1:C:323:TRP:C	1:C:327:LYS:HZ1	2.30	0.40
1:D:217:LEU:HA	1:D:222:ASP:OD2	2.21	0.40
1:D:248:THR:O	1:D:251:ILE:HG23	2.21	0.40
1:E:147:TRP:HB2	1:E:157:VAL:HG11	2.04	0.40
1:E:271:PRO:O	1:E:271:PRO:HG2	2.22	0.40
1:F:254:SER:O	1:F:257:ASP:HB3	2.22	0.40
1:F:317:LYS:HB3	1:F:317:LYS:HE3	1.51	0.40
1:G:142:LEU:HD23	1:G:142:LEU:HA	1.79	0.40
1:H:31:GLY:HA2	1:H:94:THR:HG21	2.04	0.40
1:H:327:LYS:CD	5:H:1120:HOH:O	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/331 (100%)	306 (93%)	22 (7%)	2 (1%)	21	30
1	B	331/331 (100%)	314 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	329/331 (99%)	307 (93%)	22 (7%)	0	100	100
1	D	333/331 (101%)	307 (92%)	25 (8%)	1 (0%)	36	48
1	E	330/331 (100%)	307 (93%)	21 (6%)	2 (1%)	21	30
1	F	330/331 (100%)	303 (92%)	25 (8%)	2 (1%)	21	30
1	G	332/331 (100%)	311 (94%)	20 (6%)	1 (0%)	36	48
1	H	331/331 (100%)	306 (92%)	23 (7%)	2 (1%)	21	30
All	All	2646/2648 (100%)	2461 (93%)	175 (7%)	10 (0%)	30	40

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	E	192	HIS
1	D	221	ALA
1	E	312	GLU
1	A	104	SER
1	F	221	ALA
1	F	321	THR
1	G	285	ASP
1	H	15	GLU
1	H	100	GLN

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	285/284 (100%)	243 (85%)	42 (15%)	3	3
1	B	286/284 (101%)	257 (90%)	29 (10%)	7	10
1	C	284/284 (100%)	244 (86%)	40 (14%)	3	4
1	D	288/284 (101%)	245 (85%)	43 (15%)	3	3
1	E	285/284 (100%)	238 (84%)	47 (16%)	2	2
1	F	285/284 (100%)	250 (88%)	35 (12%)	4	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	287/284 (101%)	248 (86%)	39 (14%)	3	4
1	H	286/284 (101%)	243 (85%)	43 (15%)	3	3
All	All	2286/2272 (101%)	1968 (86%)	318 (14%)	3	4

All (318) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	15	GLU
1	A	17	VAL
1	A	50	VAL
1	A	56	LYS
1	A	89	LYS
1	A	93	ILE
1	A	100	GLN
1	A	103	GLU
1	A	105	ARG
1	A	107	ASN
1	A	108	LEU
1	A	111	ARG
1	A	122	ASN
1	A	123	VAL
1	A	124	VAL
1	A	131	LYS
1	A	133	LEU
1	A	136	SER
1	A	141	ILE
1	A	177	LEU
1	A	182	LEU
1	A	189	LEU
1	A	208	VAL
1	A	219	THR
1	A	223	LYS
1	A	228	GLN
1	A	234	VAL
1	A	241	ILE
1	A	272	ILE
1	A	276	LEU
1	A	279	LEU
1	A	283	LYS
1	A	286	VAL

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Mol	Chain	Res	Type
1	A	289	SER
1	A	316	LYS
1	A	317	LYS
1	A	321	THR
1	A	322	LEU
1	A	327	LYS
1	A	329	LEU
1	A	330	GLN
1	B	7	LEU
1	B	13	LYS
1	B	15	GLU
1	B	16	HIS
1	B	19	GLN
1	B	50	VAL
1	B	68	SER
1	B	85	THR
1	B	123	VAL
1	B	124	VAL
1	B	133	LEU
1	B	173	MET
1	B	175	GLU
1	B	177	LEU
1	B	182	LEU
1	B	213	LEU
1	B	223	LYS
1	B	243	LEU
1	B	254	SER
1	B	266	LEU
1	B	276	LEU
1	B	279	LEU
1	B	283	LYS
1	B	290	VAL
1	B	296	GLN
1	B	310	GLU
1	B	315	LEU
1	B	328	GLU
1	B	331	PHE
1	C	7	LEU
1	C	13	LYS
1	C	14	GLU
1	C	17	VAL
1	C	22	ILE

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Mol	Chain	Res	Type
1	C	50	VAL
1	C	68	SER
1	C	80	LYS
1	C	84	VAL
1	C	85	THR
1	C	93	ILE
1	C	113	VAL
1	C	115	ILE
1	C	117	LYS
1	C	124	VAL
1	C	170	ARG
1	C	175	GLU
1	C	177	LEU
1	C	182	LEU
1	C	203	MET
1	C	208	VAL
1	C	210	LEU
1	C	213	LEU
1	C	222	ASP
1	C	223	LYS
1	C	224	GLU
1	C	234	VAL
1	C	276	LEU
1	C	277	LYS
1	C	279	LEU
1	C	283	LYS
1	C	284	GLU
1	C	286	VAL
1	C	290	VAL
1	C	304	LYS
1	C	310	GLU
1	C	317	LYS
1	C	326	GLN
1	C	327	LYS
1	C	329	LEU
1	D	11	LEU
1	D	12	LEU
1	D	15	GLU
1	D	17	VAL
1	D	43	LEU
1	D	58	LYS
1	D	85	THR

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Mol	Chain	Res	Type
1	D	98	ARG
1	D	103	GLU
1	D	123	VAL
1	D	124	VAL
1	D	127	SER
1	D	136	SER
1	D	141	ILE
1	D	160	SER
1	D	173	MET
1	D	177	LEU
1	D	182	LEU
1	D	189	LEU
1	D	197	VAL
1	D	204	ASN
1	D	208	VAL
1	D	209	SER
1	D	210	LEU
1	D	212	THR
1	D	228	GLN
1	D	234	VAL
1	D	236	SER
1	D	248	THR
1	D	254	SER
1	D	264[A]	LYS
1	D	264[B]	LYS
1	D	275	MET
1	D	276	LEU
1	D	279	LEU
1	D	282	ILE
1	D	283	LYS
1	D	290	VAL
1	D	304	LYS
1	D	308	THR
1	D	309	SER
1	D	322	LEU
1	D	329	LEU
1	E	5[A]	ASP
1	E	5[B]	ASP
1	E	8	ILE
1	E	13	LYS
1	E	14	GLU
1	E	15	GLU

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Mol	Chain	Res	Type
1	E	27	VAL
1	E	50	VAL
1	E	54	GLU
1	E	72	ARG
1	E	75	LYS
1	E	81	ASP
1	E	85	THR
1	E	98	ARG
1	E	99	GLN
1	E	106	LEU
1	E	108	LEU
1	E	123	VAL
1	E	124	VAL
1	E	131	LYS
1	E	133	LEU
1	E	154	LYS
1	E	160	SER
1	E	177	LEU
1	E	182	LEU
1	E	189	LEU
1	E	209	SER
1	E	212	THR
1	E	213	LEU
1	E	219	THR
1	E	223	LYS
1	E	231	LYS
1	E	234	VAL
1	E	251	ILE
1	E	276	LEU
1	E	282	ILE
1	E	283	LYS
1	E	290	VAL
1	E	301	ASP
1	E	310	GLU
1	E	315	LEU
1	E	316	LYS
1	E	317	LYS
1	E	318	SER
1	E	321	THR
1	E	330	GLN
1	E	331	PHE
1	F	11	LEU

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Mol	Chain	Res	Type
1	F	13	LYS
1	F	14	GLU
1	F	16	HIS
1	F	17	VAL
1	F	19	GLN
1	F	21	LYS
1	F	50	VAL
1	F	72	ARG
1	F	89	LYS
1	F	123	VAL
1	F	133	LEU
1	F	165	ASP
1	F	177	LEU
1	F	188	ILE
1	F	194	ASP
1	F	216	GLU
1	F	220	ASP
1	F	227	LYS
1	F	239	GLU
1	F	242	LYS
1	F	243	LEU
1	F	247	THR
1	F	272	ILE
1	F	276	LEU
1	F	279	LEU
1	F	283	LYS
1	F	286	VAL
1	F	316	LYS
1	F	317	LYS
1	F	318	SER
1	F	322	LEU
1	F	327	LYS
1	F	329	LEU
1	F	330	GLN
1	G	7	LEU
1	G	12	LEU
1	G	13	LYS
1	G	14	GLU
1	G	15	GLU
1	G	17	VAL
1	G	49	LEU
1	G	50	VAL

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Mol	Chain	Res	Type
1	G	80	LYS
1	G	89	LYS
1	G	123	VAL
1	G	124	VAL
1	G	133	LEU
1	G	154	LYS
1	G	177	LEU
1	G	182	LEU
1	G	189	LEU
1	G	203	MET
1	G	208	VAL
1	G	209	SER
1	G	211	LYS
1	G	216	GLU
1	G	217	LEU
1	G	220	ASP
1	G	223	LYS
1	G	242	LYS
1	G	248	THR
1	G	276	LEU
1	G	277	LYS
1	G	286	VAL
1	G	288	LEU
1	G	290	VAL
1	G	299	ILE
1	G	302	VAL
1	G	312[A]	GLU
1	G	312[B]	GLU
1	G	320	ASP
1	G	325	ILE
1	G	327	LYS
1	H	11	LEU
1	H	14	GLU
1	H	23	THR
1	H	50	VAL
1	H	85	THR
1	H	89	LYS
1	H	94	THR
1	H	100	GLN
1	H	103	GLU
1	H	104	SER
1	H	105	ARG

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Mol	Chain	Res	Type
1	H	107	ASN
1	H	108	LEU
1	H	124	VAL
1	H	127	SER
1	H	133	LEU
1	H	154	LYS
1	H	170	ARG
1	H	177	LEU
1	H	182	LEU
1	H	189	LEU
1	H	208	VAL
1	H	209	SER
1	H	210	LEU
1	H	211	LYS
1	H	216	GLU
1	H	248	THR
1	H	272	ILE
1	H	273	SER
1	H	276	LEU
1	H	283	LYS
1	H	286	VAL
1	H	290	VAL
1	H	309	SER
1	H	310	GLU
1	H	311	GLU
1	H	314	HIS
1	H	316	LYS
1	H	317	LYS
1	H	320	ASP
1	H	322	LEU
1	H	327	LYS
1	H	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	16	HIS
1	A	19	GLN
1	A	20	ASN
1	A	112	ASN
1	A	122	ASN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	296	GLN
1	A	314	HIS
1	A	326	GLN
1	A	330	GLN
1	B	20	ASN
1	B	107	ASN
1	B	110	GLN
1	B	112	ASN
1	B	137	ASN
1	B	204	ASN
1	B	230	HIS
1	B	297	ASN
1	C	6	GLN
1	C	10	ASN
1	C	87	ASN
1	C	99	GLN
1	C	112	ASN
1	C	114	ASN
1	C	204	ASN
1	C	230	HIS
1	C	297	ASN
1	D	6	GLN
1	D	10	ASN
1	D	20	ASN
1	D	99	GLN
1	D	112	ASN
1	D	204	ASN
1	D	230	HIS
1	D	296	GLN
1	D	297	ASN
1	D	326	GLN
1	E	6	GLN
1	E	10	ASN
1	E	107	ASN
1	E	110	GLN
1	E	297	ASN
1	E	314	HIS
1	E	330	GLN
1	F	107	ASN
1	F	112	ASN
1	F	192	HIS

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Mol	Chain	Res	Type
1	F	204	ASN
1	F	230	HIS
1	F	232	GLN
1	F	297	ASN
1	G	6	GLN
1	G	9	HIS
1	G	87	ASN
1	G	100	GLN
1	G	112	ASN
1	G	114	ASN
1	G	204	ASN
1	G	232	GLN
1	H	16	HIS
1	H	19	GLN
1	H	100	GLN
1	H	204	ASN
1	H	297	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](#)

39 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAI	G	332	-	47,48,48	1.42	8 (17%)	64,73,73	2.35	24 (37%)
4	ACT	G	334	-	3,3,3	0.70	0	3,3,3	1.86	1 (33%)
4	ACT	E	335	-	3,3,3	1.08	0	3,3,3	2.03	2 (66%)
4	ACT	D	337	-	3,3,3	1.02	0	3,3,3	0.86	0
4	ACT	C	334	-	3,3,3	0.98	0	3,3,3	2.25	2 (66%)
4	ACT	D	336	-	3,3,3	1.01	0	3,3,3	1.13	0
4	ACT	F	335	-	3,3,3	0.92	0	3,3,3	1.88	1 (33%)
4	ACT	H	334	-	3,3,3	0.82	0	3,3,3	1.54	0
2	NAI	A	332	-	47,48,48	1.95	6 (12%)	64,73,73	1.98	19 (29%)
4	ACT	E	336	-	3,3,3	0.96	0	3,3,3	1.64	1 (33%)
3	OXM	F	333	-	5,5,5	2.54	1 (20%)	2,6,6	1.42	0
4	ACT	H	336	-	3,3,3	1.06	0	3,3,3	1.42	0
2	NAI	D	332	-	47,48,48	2.08	13 (27%)	64,73,73	2.10	20 (31%)
2	NAI	F	332	-	47,48,48	1.56	7 (14%)	64,73,73	2.04	23 (35%)
3	OXM	B	333	-	5,5,5	3.80	2 (40%)	2,6,6	0.44	0
3	OXM	C	333	-	5,5,5	2.84	1 (20%)	2,6,6	0.78	0
4	ACT	E	338	-	3,3,3	0.94	0	3,3,3	1.86	1 (33%)
3	OXM	H	333	-	5,5,5	2.53	1 (20%)	2,6,6	1.37	0
4	ACT	F	334	-	3,3,3	0.94	0	3,3,3	1.06	0
4	ACT	G	335	-	3,3,3	0.76	0	3,3,3	1.74	2 (66%)
2	NAI	H	332	-	47,48,48	1.59	7 (14%)	64,73,73	2.20	22 (34%)
3	OXM	A	333	-	5,5,5	3.68	1 (20%)	2,6,6	1.12	0
4	ACT	E	334	-	3,3,3	1.09	0	3,3,3	0.90	0
2	NAI	B	332	-	47,48,48	1.67	7 (14%)	64,73,73	2.18	23 (35%)
4	ACT	D	334	-	3,3,3	1.04	0	3,3,3	1.11	0
4	ACT	D	338	-	3,3,3	1.09	0	3,3,3	0.88	0
4	ACT	E	337	-	3,3,3	1.34	0	3,3,3	0.90	0
4	ACT	D	335	-	3,3,3	0.93	0	3,3,3	1.62	1 (33%)
4	ACT	H	337	-	3,3,3	0.83	0	3,3,3	1.72	2 (66%)
2	NAI	E	332	-	47,48,48	1.97	8 (17%)	64,73,73	1.84	14 (21%)
4	ACT	G	336	-	3,3,3	1.00	0	3,3,3	1.70	2 (66%)
4	ACT	C	335	-	3,3,3	1.10	0	3,3,3	1.65	1 (33%)
4	ACT	A	334	-	3,3,3	1.25	0	3,3,3	1.59	1 (33%)
3	OXM	G	333	-	5,5,5	3.80	1 (20%)	2,6,6	1.06	0
3	OXM	E	333	-	5,5,5	2.42	1 (20%)	2,6,6	1.54	1 (50%)
4	ACT	H	335	-	3,3,3	0.89	0	3,3,3	1.50	0
4	ACT	B	334	-	3,3,3	1.19	0	3,3,3	1.89	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXM	D	333	-	5,5,5	3.04	1 (20%)	2,6,6	0.61	0
2	NAI	C	332	-	47,48,48	1.54	7 (14%)	64,73,73	2.08	21 (32%)

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	OXM	H	333	-	-	4/4/4/4	-
2	NAI	D	332	-	-	8/29/72/72	0/5/5/5
2	NAI	F	332	-	-	8/29/72/72	0/5/5/5
2	NAI	H	332	-	-	8/29/72/72	0/5/5/5
3	OXM	A	333	-	-	0/4/4/4	-
2	NAI	G	332	-	-	12/29/72/72	0/5/5/5
3	OXM	B	333	-	-	0/4/4/4	-
3	OXM	C	333	-	-	0/4/4/4	-
2	NAI	B	332	-	-	5/29/72/72	0/5/5/5
3	OXM	G	333	-	-	0/4/4/4	-
3	OXM	E	333	-	-	3/4/4/4	-
3	OXM	F	333	-	-	0/4/4/4	-
3	OXM	D	333	-	-	0/4/4/4	-
2	NAI	A	332	-	-	4/29/72/72	0/5/5/5
2	NAI	C	332	-	-	5/29/72/72	0/5/5/5
2	NAI	E	332	-	-	10/29/72/72	0/5/5/5

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	333	OXM	C1-C2	-8.30	1.45	1.55
3	B	333	OXM	C1-C2	-8.03	1.46	1.55
3	A	333	OXM	C1-C2	-7.92	1.46	1.55
2	A	332	NAI	PA-O3	7.56	1.67	1.59
3	D	333	OXM	C1-C2	-6.46	1.47	1.55
2	D	332	NAI	PA-O3	6.39	1.66	1.59
2	E	332	NAI	PN-O3	6.28	1.66	1.59
2	B	332	NAI	C4N-C3N	-6.06	1.38	1.50
3	C	333	OXM	C1-C2	-5.97	1.48	1.55
2	E	332	NAI	C4N-C3N	-5.83	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	332	NAI	PN-O3	5.76	1.65	1.59
2	D	332	NAI	PN-O3	5.69	1.65	1.59
2	F	332	NAI	C4N-C3N	-5.66	1.39	1.50
2	H	332	NAI	C4N-C3N	-5.44	1.39	1.50
2	D	332	NAI	O7N-C7N	5.31	1.36	1.24
2	A	332	NAI	C4N-C3N	-5.31	1.40	1.50
3	F	333	OXM	C1-C2	-5.20	1.49	1.55
2	E	332	NAI	PA-O3	5.12	1.65	1.59
3	H	333	OXM	C1-C2	-5.10	1.49	1.55
2	D	332	NAI	C4N-C3N	-5.07	1.40	1.50
3	E	333	OXM	C1-C2	-4.94	1.49	1.55
2	C	332	NAI	C4N-C3N	-4.80	1.40	1.50
2	E	332	NAI	O7N-C7N	4.52	1.35	1.24
2	G	332	NAI	C4N-C3N	-4.51	1.41	1.50
2	B	332	NAI	O7N-C7N	4.35	1.34	1.24
2	C	332	NAI	O7N-C7N	4.23	1.34	1.24
2	F	332	NAI	C4N-C5N	-4.21	1.38	1.49
2	A	332	NAI	O7N-C7N	4.12	1.34	1.24
2	F	332	NAI	O7N-C7N	3.69	1.33	1.24
2	H	332	NAI	O7N-C7N	3.67	1.33	1.24
2	H	332	NAI	C4A-N9A	-3.45	1.30	1.37
2	C	332	NAI	C4N-C5N	-3.40	1.40	1.49
2	H	332	NAI	C4N-C5N	-3.37	1.40	1.49
2	B	332	NAI	C4N-C5N	-3.24	1.40	1.49
2	G	332	NAI	O7N-C7N	3.11	1.31	1.24
2	C	332	NAI	C4A-N9A	-3.11	1.31	1.37
2	E	332	NAI	C4N-C5N	-3.00	1.41	1.49
2	A	332	NAI	C4N-C5N	-3.00	1.41	1.49
2	G	332	NAI	C8A-N9A	-2.99	1.32	1.37
2	E	332	NAI	C8A-N7A	2.88	1.37	1.31
2	F	332	NAI	PN-O3	2.81	1.62	1.59
2	D	332	NAI	C4N-C5N	-2.77	1.41	1.49
2	F	332	NAI	C8A-N7A	2.71	1.36	1.31
2	D	332	NAI	C6N-C5N	2.64	1.41	1.33
2	B	332	NAI	C4A-N9A	-2.59	1.32	1.37
2	C	332	NAI	PA-O3	2.58	1.62	1.59
2	G	332	NAI	C5A-N7A	-2.48	1.34	1.39
2	D	332	NAI	C2N-C3N	2.46	1.41	1.35
2	H	332	NAI	C6N-C5N	2.46	1.40	1.33
2	H	332	NAI	C8A-N7A	2.43	1.36	1.31
2	B	332	NAI	C8A-N7A	2.43	1.36	1.31
2	H	332	NAI	C7N-N7N	-2.32	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	332	NAI	C7N-N7N	-2.29	1.26	1.33
2	E	332	NAI	C4A-N3A	2.28	1.38	1.34
2	D	332	NAI	C8A-N7A	2.27	1.36	1.31
2	B	332	NAI	PN-O3	-2.25	1.57	1.59
2	B	332	NAI	C6N-C5N	2.22	1.39	1.33
2	D	332	NAI	C2A-N3A	2.21	1.37	1.33
2	G	332	NAI	C4N-C5N	-2.18	1.43	1.49
2	C	332	NAI	C7N-N7N	-2.16	1.27	1.33
2	C	332	NAI	PN-O3	2.15	1.61	1.59
2	G	332	NAI	C4A-N3A	2.11	1.38	1.34
2	G	332	NAI	C6N-C5N	2.07	1.39	1.33
2	F	332	NAI	O4D-C4D	-2.06	1.40	1.45
2	D	332	NAI	C4A-N3A	2.04	1.38	1.34
3	B	333	OXM	O2-C2	2.03	1.27	1.22
2	G	332	NAI	C7N-N7N	-2.03	1.27	1.33
2	D	332	NAI	C6A-N6A	2.03	1.39	1.34
2	A	332	NAI	C8A-N7A	2.03	1.35	1.31
2	D	332	NAI	O4D-C1D	2.02	1.46	1.42
2	E	332	NAI	C6N-C5N	2.02	1.39	1.33
2	F	332	NAI	C4A-N9A	-2.01	1.33	1.37

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	332	NAI	N3A-C2A-N1A	-6.69	118.45	128.58
2	F	332	NAI	N3A-C2A-N1A	-6.43	118.85	128.58
2	G	332	NAI	O2A-PA-O3	6.07	123.69	107.27
2	C	332	NAI	N3A-C2A-N1A	-5.71	119.94	128.58
2	D	332	NAI	C5A-C4A-N3A	-5.67	118.90	126.72
2	G	332	NAI	N3A-C2A-N1A	-5.62	120.08	128.58
2	G	332	NAI	C4A-N9A-C8A	5.36	111.37	105.74
2	H	332	NAI	C1D-N1N-C2N	-5.33	112.36	121.14
2	H	332	NAI	N3A-C2A-N1A	-5.28	120.58	128.58
2	E	332	NAI	N3A-C2A-N1A	-5.24	120.66	128.58
2	C	332	NAI	N9A-C8A-N7A	-5.20	106.56	113.94
2	H	332	NAI	C4A-N9A-C8A	5.13	111.12	105.74
2	B	332	NAI	N9A-C8A-N7A	-5.13	106.66	113.94
2	G	332	NAI	N9A-C8A-N7A	-5.09	106.72	113.94
2	H	332	NAI	O3-PA-O1A	-4.94	95.85	110.70
2	H	332	NAI	N9A-C8A-N7A	-4.93	106.94	113.94
2	E	332	NAI	N9A-C8A-N7A	-4.86	107.03	113.94
2	A	332	NAI	N3A-C2A-N1A	-4.86	121.23	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	332	NAI	C5A-C4A-N3A	-4.85	120.04	126.72
2	B	332	NAI	C4A-N9A-C8A	4.83	110.81	105.74
2	H	332	NAI	C2B-C1B-N9A	-4.63	101.80	113.30
2	E	332	NAI	C4A-N9A-C8A	4.47	110.43	105.74
2	E	332	NAI	C5A-C4A-N3A	-4.46	120.57	126.72
2	C	332	NAI	C4A-N9A-C8A	4.45	110.41	105.74
2	D	332	NAI	C4B-O4B-C1B	-4.36	99.84	109.47
2	A	332	NAI	N3A-C4A-N9A	4.28	134.44	127.17
2	G	332	NAI	C1D-N1N-C2N	-4.28	114.10	121.14
2	F	332	NAI	N9A-C8A-N7A	-4.24	107.92	113.94
2	D	332	NAI	N9A-C8A-N7A	-4.22	107.95	113.94
2	D	332	NAI	N3A-C4A-N9A	4.13	134.20	127.17
2	C	332	NAI	C5A-C4A-N3A	-3.99	121.22	126.72
2	B	332	NAI	O4B-C1B-N9A	3.98	115.73	108.09
2	A	332	NAI	C4A-N9A-C8A	3.92	109.85	105.74
2	G	332	NAI	C5A-C4A-N3A	-3.90	121.34	126.72
2	D	332	NAI	C3N-C7N-N7N	-3.85	110.83	117.67
2	H	332	NAI	O2A-PA-O3	3.82	117.60	107.27
2	E	332	NAI	N3A-C4A-N9A	3.80	133.63	127.17
2	F	332	NAI	C4A-N9A-C8A	3.80	109.72	105.74
2	C	332	NAI	C4A-N9A-C1B	-3.77	117.82	126.63
2	F	332	NAI	O4B-C1B-N9A	3.75	115.30	108.09
2	G	332	NAI	C5A-N7A-C8A	3.72	109.30	103.45
2	F	332	NAI	C2A-N3A-C4A	3.72	120.91	111.83
2	D	332	NAI	C5A-N7A-C8A	3.68	109.23	103.45
2	B	332	NAI	C2A-N3A-C4A	3.64	120.72	111.83
2	D	332	NAI	C5D-C4D-C3D	-3.64	102.12	115.21
2	A	332	NAI	C6N-N1N-C2N	3.64	123.21	119.32
2	F	332	NAI	C5A-C4A-N3A	-3.62	121.73	126.72
2	C	332	NAI	C2A-N3A-C4A	3.61	120.64	111.83
2	G	332	NAI	N3A-C4A-N9A	3.59	133.28	127.17
2	F	332	NAI	C4A-N9A-C1B	-3.56	118.31	126.63
2	E	332	NAI	C1D-N1N-C2N	-3.56	115.28	121.14
2	A	332	NAI	N9A-C8A-N7A	-3.55	108.90	113.94
2	B	332	NAI	O2B-C2B-C1B	-3.55	97.89	110.10
2	D	332	NAI	C4A-C5A-N7A	-3.51	106.56	110.58
2	D	332	NAI	O7N-C7N-C3N	3.50	127.49	120.90
2	E	332	NAI	C2A-N3A-C4A	3.48	120.32	111.83
2	A	332	NAI	C5B-C4B-C3B	-3.44	102.83	115.21
2	D	332	NAI	C4A-N9A-C8A	3.43	109.34	105.74
2	D	332	NAI	N3A-C2A-N1A	-3.42	123.40	128.58
2	G	332	NAI	C6N-N1N-C2N	3.41	122.97	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	332	NAI	C5A-C4A-N3A	-3.39	122.05	126.72
2	B	332	NAI	O3D-C3D-C4D	-3.37	101.39	111.08
2	C	332	NAI	C1D-N1N-C2N	-3.34	115.63	121.14
2	B	332	NAI	C4A-N9A-C1B	-3.33	118.84	126.63
2	B	332	NAI	C5A-C4A-N3A	-3.33	122.13	126.72
2	C	332	NAI	C4A-C5A-N7A	-3.31	106.80	110.58
2	H	332	NAI	C4B-O4B-C1B	-3.24	102.32	109.47
2	G	332	NAI	O4D-C1D-N1N	3.23	114.25	108.08
2	A	332	NAI	C2A-N3A-C4A	3.22	119.70	111.83
2	G	332	NAI	O7N-C7N-C3N	-3.20	114.86	120.90
2	H	332	NAI	C6N-N1N-C2N	3.19	122.73	119.32
2	G	332	NAI	C2A-N3A-C4A	3.16	119.55	111.83
2	C	332	NAI	C5A-N7A-C8A	3.16	108.42	103.45
2	F	332	NAI	O4D-C1D-N1N	3.08	113.96	108.08
2	A	332	NAI	O5B-C5B-C4B	-3.06	98.56	108.99
2	B	332	NAI	C4B-O4B-C1B	-3.05	102.72	109.47
2	D	332	NAI	C2A-N3A-C4A	3.04	119.25	111.83
2	E	332	NAI	C5A-N7A-C8A	3.03	108.22	103.45
2	G	332	NAI	O3-PA-O1A	-3.01	101.64	110.70
2	D	332	NAI	C2B-C1B-N9A	3.00	120.76	113.30
2	C	332	NAI	C4B-O4B-C1B	-2.99	102.88	109.47
2	E	332	NAI	C5A-C6A-N6A	-2.97	115.94	123.29
2	G	332	NAI	C4A-C5A-N7A	-2.93	107.23	110.58
4	C	334	ACT	OXT-C-O	-2.88	111.33	122.03
2	H	332	NAI	O3D-C3D-C4D	-2.88	102.81	111.08
2	C	332	NAI	O4D-C1D-N1N	2.87	113.56	108.08
2	G	332	NAI	C3N-C7N-N7N	2.86	122.75	117.67
2	G	332	NAI	C4B-O4B-C1B	-2.84	103.19	109.47
2	C	332	NAI	C6N-N1N-C2N	2.83	122.34	119.32
2	H	332	NAI	C3N-C2N-N1N	-2.83	119.06	123.20
2	D	332	NAI	O1N-PN-O3	2.82	114.89	107.27
2	C	332	NAI	C3N-C7N-N7N	2.81	122.67	117.67
2	H	332	NAI	O1N-PN-O2N	2.81	125.51	112.44
2	C	332	NAI	O3-PA-O1A	-2.81	102.26	110.70
4	E	335	ACT	OXT-C-O	-2.79	111.68	122.03
2	A	332	NAI	O5B-PA-O1A	-2.79	97.89	108.94
2	B	332	NAI	C5A-N7A-C8A	2.76	107.79	103.45
2	H	332	NAI	C2A-N3A-C4A	2.74	118.53	111.83
2	E	332	NAI	C4B-O4B-C1B	-2.73	103.44	109.47
2	G	332	NAI	O5B-C5B-C4B	-2.69	99.84	108.99
2	B	332	NAI	O5B-C5B-C4B	-2.68	99.87	108.99
2	F	332	NAI	O5B-C5B-C4B	-2.66	99.93	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	335	ACT	OXT-C-O	-2.65	112.20	122.03
2	F	332	NAI	O4D-C1D-C2D	-2.63	101.00	106.62
4	C	334	ACT	OXT-C-CH3	2.62	126.03	115.05
2	G	332	NAI	O2A-PA-O5B	-2.60	95.80	107.57
2	A	332	NAI	N6A-C6A-N1A	2.60	124.16	118.38
4	G	334	ACT	OXT-C-CH3	2.59	125.89	115.05
2	D	332	NAI	C6A-C5A-C4A	2.58	120.70	117.18
2	B	332	NAI	C5B-C4B-C3B	-2.58	105.93	115.21
2	A	332	NAI	C5A-C6A-N6A	-2.57	116.93	123.29
2	A	332	NAI	C4B-O4B-C1B	-2.57	103.80	109.47
2	B	332	NAI	O4B-C4B-C3B	2.56	110.24	105.15
2	D	332	NAI	O5B-C5B-C4B	-2.55	100.29	108.99
4	E	338	ACT	OXT-C-O	-2.55	112.58	122.03
2	F	332	NAI	C1D-N1N-C2N	-2.54	116.95	121.14
2	A	332	NAI	O1N-PN-O3	2.52	114.08	107.27
2	C	332	NAI	O2A-PA-O3	2.51	114.06	107.27
2	C	332	NAI	C6A-C5A-N7A	2.50	136.91	132.09
2	F	332	NAI	O3-PA-O1A	-2.50	103.19	110.70
2	G	332	NAI	O1N-PN-O2N	2.49	124.05	112.44
2	H	332	NAI	O2A-PA-O1A	2.49	124.03	112.44
2	D	332	NAI	O3-PN-O2N	-2.48	103.25	110.70
2	F	332	NAI	C4A-C5A-N7A	-2.47	107.76	110.58
2	G	332	NAI	O3-PN-O2N	-2.46	103.32	110.70
2	F	332	NAI	C2A-N1A-C6A	2.45	122.75	118.73
2	A	332	NAI	C2D-C1D-N1N	-2.44	107.31	113.31
2	F	332	NAI	O7N-C7N-C3N	-2.44	116.31	120.90
2	A	332	NAI	O2A-PA-O1A	2.43	123.75	112.44
2	B	332	NAI	C2D-C3D-C4D	2.40	107.25	102.61
2	B	332	NAI	C4A-C5A-N7A	-2.40	107.84	110.58
2	G	332	NAI	C3N-C2N-N1N	-2.39	119.70	123.20
2	H	332	NAI	O5B-C5B-C4B	-2.39	100.86	108.99
2	F	332	NAI	O2A-PA-O3	2.39	113.73	107.27
2	A	332	NAI	C5A-N7A-C8A	2.39	107.20	103.45
4	B	334	ACT	OXT-C-O	-2.38	113.18	122.03
2	F	332	NAI	O3D-C3D-C2D	-2.38	104.18	111.82
4	C	335	ACT	OXT-C-O	-2.38	113.20	122.03
2	C	332	NAI	C2D-C3D-C4D	2.38	107.20	102.61
2	G	332	NAI	N6A-C6A-N1A	2.37	123.65	118.38
2	B	332	NAI	C5D-C4D-C3D	-2.36	106.73	115.21
2	C	332	NAI	O2B-C2B-C1B	2.34	118.18	110.10
2	E	332	NAI	N6A-C6A-N1A	2.28	123.46	118.38
2	D	332	NAI	O4B-C1B-C2B	-2.27	101.75	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	332	NAI	O1N-PN-O3	2.27	113.40	107.27
2	F	332	NAI	C6A-C5A-N7A	2.26	136.45	132.09
2	H	332	NAI	N3A-C4A-N9A	2.25	131.00	127.17
2	B	332	NAI	N3A-C4A-N9A	2.25	131.00	127.17
2	C	332	NAI	N3A-C4A-N9A	2.24	130.97	127.17
4	B	334	ACT	OXT-C-CH3	2.23	124.42	115.05
2	E	332	NAI	C2D-C3D-C4D	2.23	106.92	102.61
2	B	332	NAI	C2B-C1B-N9A	-2.22	107.80	113.30
2	G	332	NAI	C2A-N1A-C6A	2.21	122.37	118.73
2	H	332	NAI	C4A-C5A-N7A	-2.21	108.05	110.58
2	H	332	NAI	C2D-C3D-C4D	2.21	106.88	102.61
2	E	332	NAI	C4A-N9A-C1B	-2.21	121.47	126.63
2	H	332	NAI	C5A-N7A-C8A	2.20	106.91	103.45
2	B	332	NAI	O4D-C1D-N1N	2.20	112.28	108.08
4	E	336	ACT	OXT-C-O	-2.20	113.86	122.03
2	F	332	NAI	C5A-N7A-C8A	2.18	106.88	103.45
2	F	332	NAI	C1B-N9A-C8A	2.18	131.94	127.09
2	D	332	NAI	O3B-C3B-C2B	2.16	118.73	111.82
4	G	335	ACT	OXT-C-O	-2.15	114.03	122.03
4	H	337	ACT	OXT-C-O	-2.15	114.05	122.03
4	A	334	ACT	OXT-C-O	-2.15	114.05	122.03
2	B	332	NAI	O5D-PN-O2N	-2.14	100.47	108.94
2	E	332	NAI	O4D-C1D-N1N	2.14	112.16	108.08
4	G	336	ACT	OXT-C-O	-2.13	114.13	122.03
3	E	333	OXM	O3-C2-O2	-2.13	118.83	123.90
2	D	332	NAI	O4D-C4D-C3D	2.12	109.35	105.15
2	F	332	NAI	C3N-C2N-N1N	-2.11	120.10	123.20
2	H	332	NAI	C2A-N1A-C6A	2.11	122.20	118.73
4	G	335	ACT	OXT-C-CH3	2.10	123.86	115.05
2	B	332	NAI	C3D-C2D-C1D	-2.10	97.49	101.46
2	G	332	NAI	C3D-C2D-C1D	-2.10	97.50	101.46
4	E	335	ACT	OXT-C-CH3	2.08	123.77	115.05
4	H	337	ACT	OXT-C-CH3	2.07	123.74	115.05
2	A	332	NAI	O3-PA-O1A	-2.07	104.47	110.70
2	C	332	NAI	C1B-N9A-C8A	2.07	131.68	127.09
2	H	332	NAI	O3B-C3B-C4B	-2.06	105.15	111.08
2	C	332	NAI	O3D-C3D-C4D	-2.05	105.20	111.08
4	D	335	ACT	OXT-C-O	-2.05	114.43	122.03
2	F	332	NAI	O1N-PN-O2N	2.03	121.90	112.44
4	G	336	ACT	OXT-C-CH3	2.03	123.57	115.05
2	B	332	NAI	O1N-PN-O2N	2.02	121.82	112.44
2	A	332	NAI	O1N-PN-O2N	2.00	121.76	112.44

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	332	NAI	O4B-C4B-C5B-O5B
2	D	332	NAI	C5D-O5D-PN-O3
2	D	332	NAI	C5D-O5D-PN-O2N
2	E	332	NAI	C5D-O5D-PN-O3
2	E	332	NAI	C5D-O5D-PN-O1N
2	E	332	NAI	C5D-O5D-PN-O2N
2	E	332	NAI	O4D-C4D-C5D-O5D
2	F	332	NAI	C5B-O5B-PA-O1A
2	F	332	NAI	C5B-O5B-PA-O3
2	G	332	NAI	C5B-O5B-PA-O3
3	E	333	OXM	N1-C1-C2-O3
3	E	333	OXM	O1-C1-C2-O3
3	H	333	OXM	N1-C1-C2-O2
3	H	333	OXM	N1-C1-C2-O3
3	H	333	OXM	O1-C1-C2-O3
2	E	332	NAI	C3D-C4D-C5D-O5D
2	D	332	NAI	C3B-C4B-C5B-O5B
2	G	332	NAI	O4B-C4B-C5B-O5B
2	H	332	NAI	PN-O3-PA-O1A
3	H	333	OXM	O1-C1-C2-O2
2	D	332	NAI	C2N-C3N-C7N-N7N
2	E	332	NAI	C2D-C1D-N1N-C2N
2	F	332	NAI	C2D-C1D-N1N-C6N
2	H	332	NAI	C2D-C1D-N1N-C2N
2	E	332	NAI	C2D-C1D-N1N-C6N
2	G	332	NAI	C2D-C1D-N1N-C2N
2	E	332	NAI	O4D-C1D-N1N-C2N
2	D	332	NAI	O4D-C1D-N1N-C2N
2	F	332	NAI	C2D-C1D-N1N-C2N
2	G	332	NAI	C2D-C1D-N1N-C6N
2	H	332	NAI	C2D-C1D-N1N-C6N
2	B	332	NAI	O4B-C4B-C5B-O5B
2	A	332	NAI	O4D-C1D-N1N-C2N
2	E	332	NAI	O4D-C1D-N1N-C6N
2	A	332	NAI	O4B-C4B-C5B-O5B
2	D	332	NAI	C5D-O5D-PN-O1N
2	G	332	NAI	C5B-O5B-PA-O1A
2	G	332	NAI	C5B-O5B-PA-O2A
2	H	332	NAI	O4D-C1D-N1N-C2N
2	H	332	NAI	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	G	332	NAI	PN-O3-PA-O2A
2	H	332	NAI	PN-O3-PA-O2A
2	F	332	NAI	C3D-C4D-C5D-O5D
2	H	332	NAI	C3D-C4D-C5D-O5D
2	C	332	NAI	O4D-C1D-N1N-C2N
2	G	332	NAI	O4D-C1D-N1N-C2N
2	C	332	NAI	C2D-C1D-N1N-C2N
2	F	332	NAI	O4D-C1D-N1N-C2N
3	E	333	OXM	N1-C1-C2-O2
2	B	332	NAI	O4D-C1D-N1N-C2N
2	G	332	NAI	C2N-C3N-C7N-N7N
2	D	332	NAI	C4D-C5D-O5D-PN
2	F	332	NAI	O4D-C1D-N1N-C6N
2	E	332	NAI	O4B-C4B-C5B-O5B
2	B	332	NAI	C2D-C1D-N1N-C2N
2	C	332	NAI	O4D-C1D-N1N-C6N
2	G	332	NAI	O4D-C1D-N1N-C6N
2	B	332	NAI	C3B-C4B-C5B-O5B
2	B	332	NAI	PA-O3-PN-O2N
2	G	332	NAI	PN-O3-PA-O1A
2	F	332	NAI	O4B-C4B-C5B-O5B
2	C	332	NAI	C2D-C1D-N1N-C6N
2	A	332	NAI	C2B-C1B-N9A-C8A
2	G	332	NAI	C2B-C1B-N9A-C8A
2	H	332	NAI	C2B-C1B-N9A-C8A
2	A	332	NAI	C2D-C1D-N1N-C2N
2	C	332	NAI	O4B-C4B-C5B-O5B

There are no ring outliers.

17 monomers are involved in 47 short contacts:

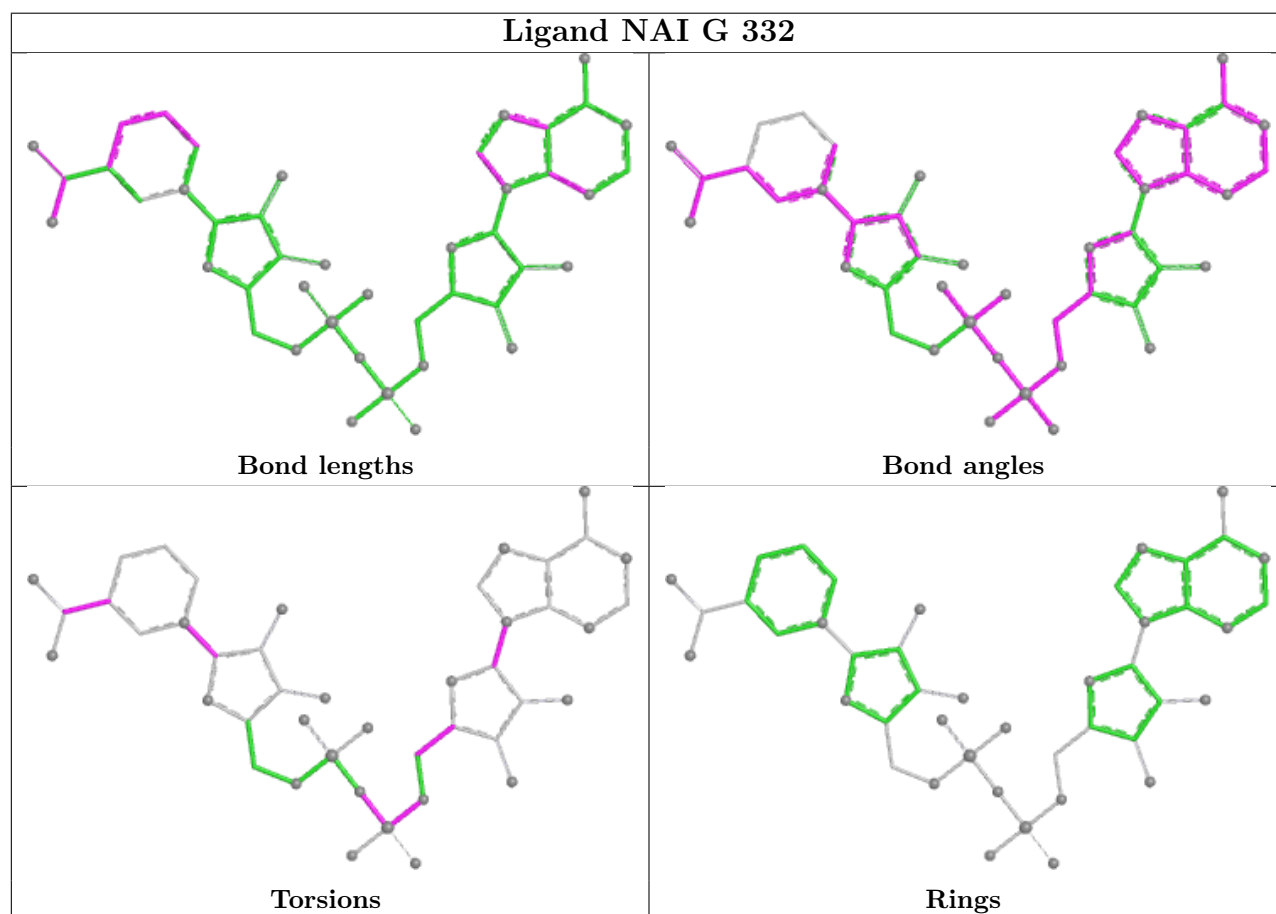
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	332	NAI	2	0
4	C	334	ACT	2	0
4	D	336	ACT	2	0
4	F	335	ACT	1	0
2	A	332	NAI	4	0
3	F	333	OXM	3	0
2	D	332	NAI	13	0
2	F	332	NAI	4	0
3	C	333	OXM	1	0
2	H	332	NAI	1	0

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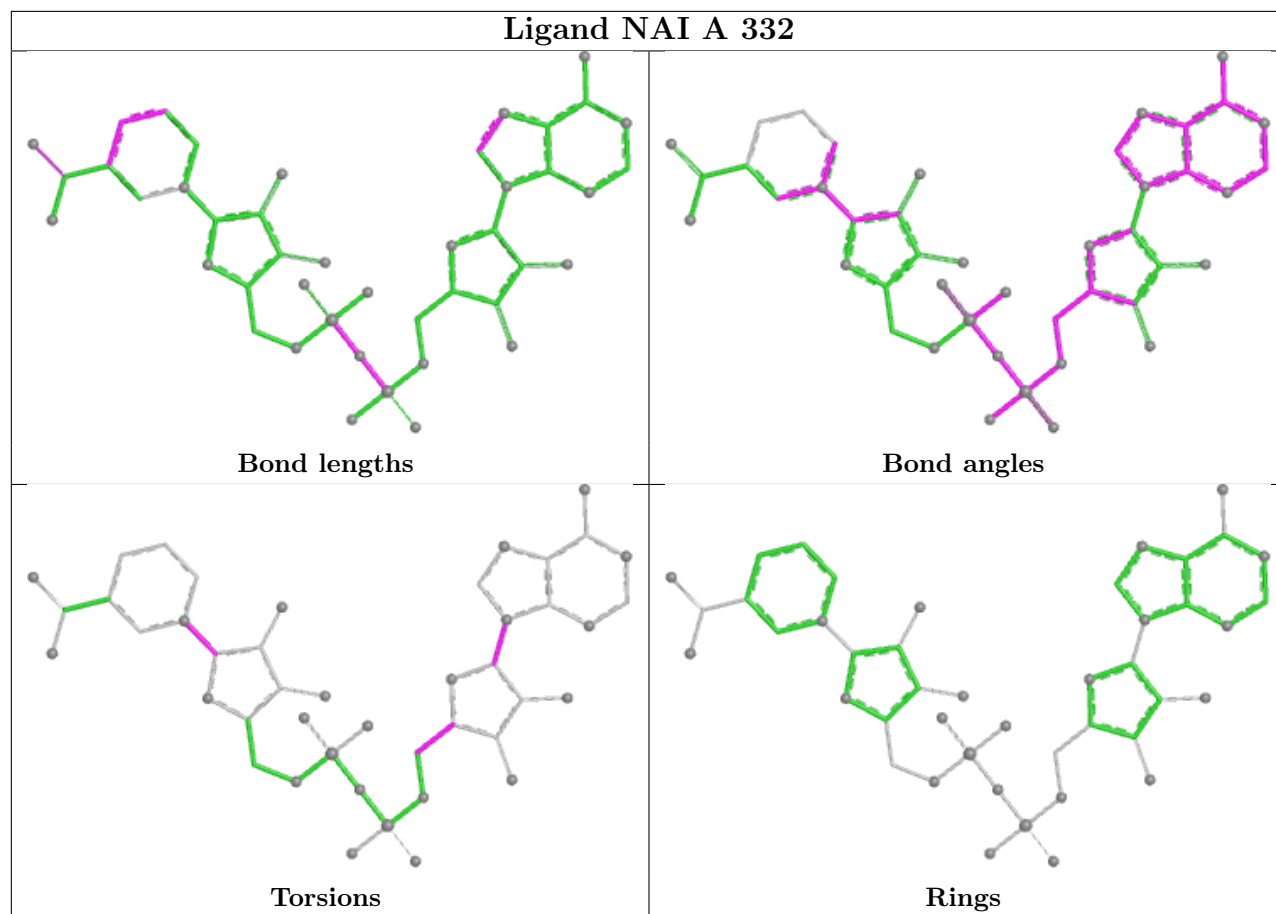
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	333	OXM	1	0
4	E	334	ACT	1	0
2	B	332	NAI	2	0
2	E	332	NAI	9	0
3	G	333	OXM	1	0
3	E	333	OXM	1	0
2	C	332	NAI	4	0

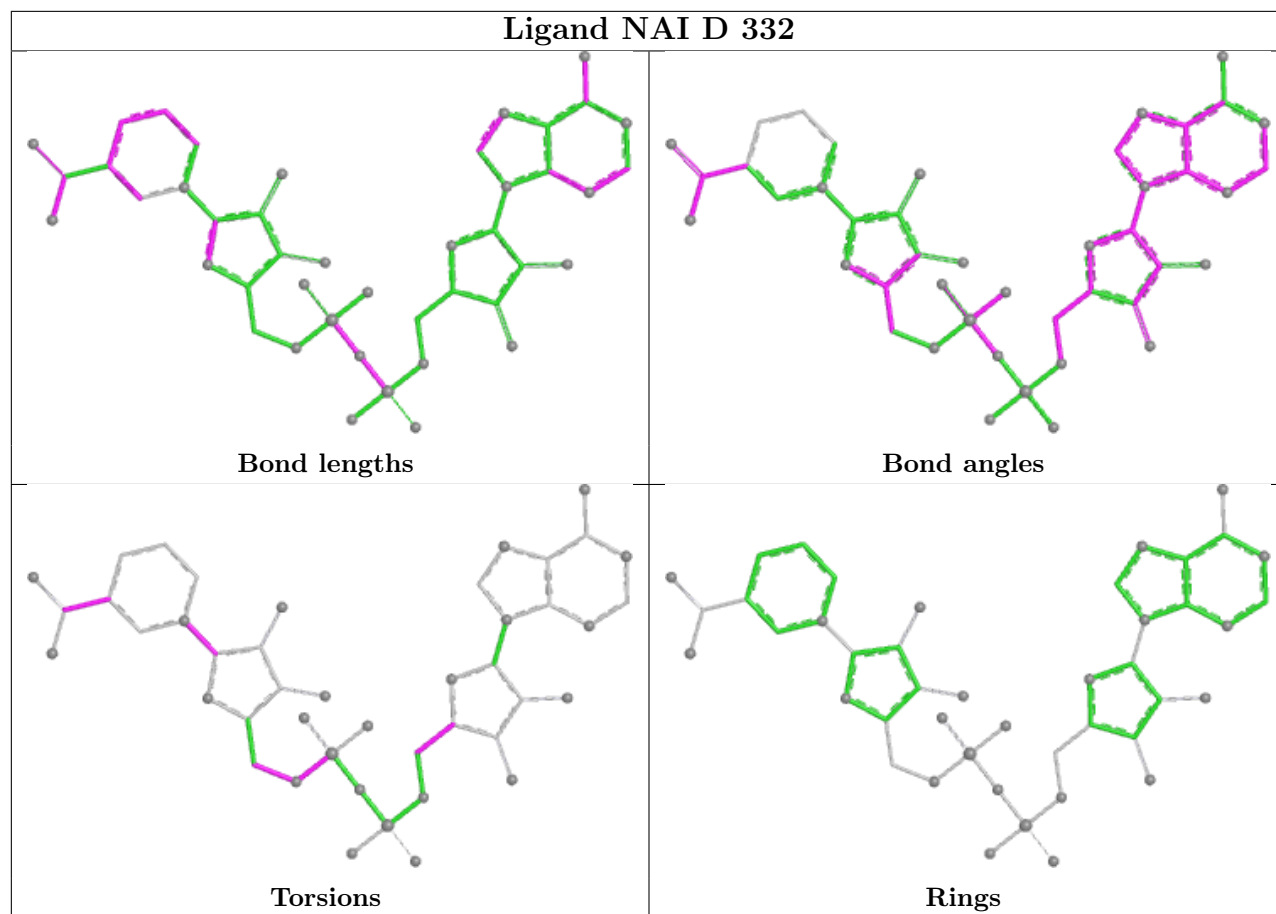
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



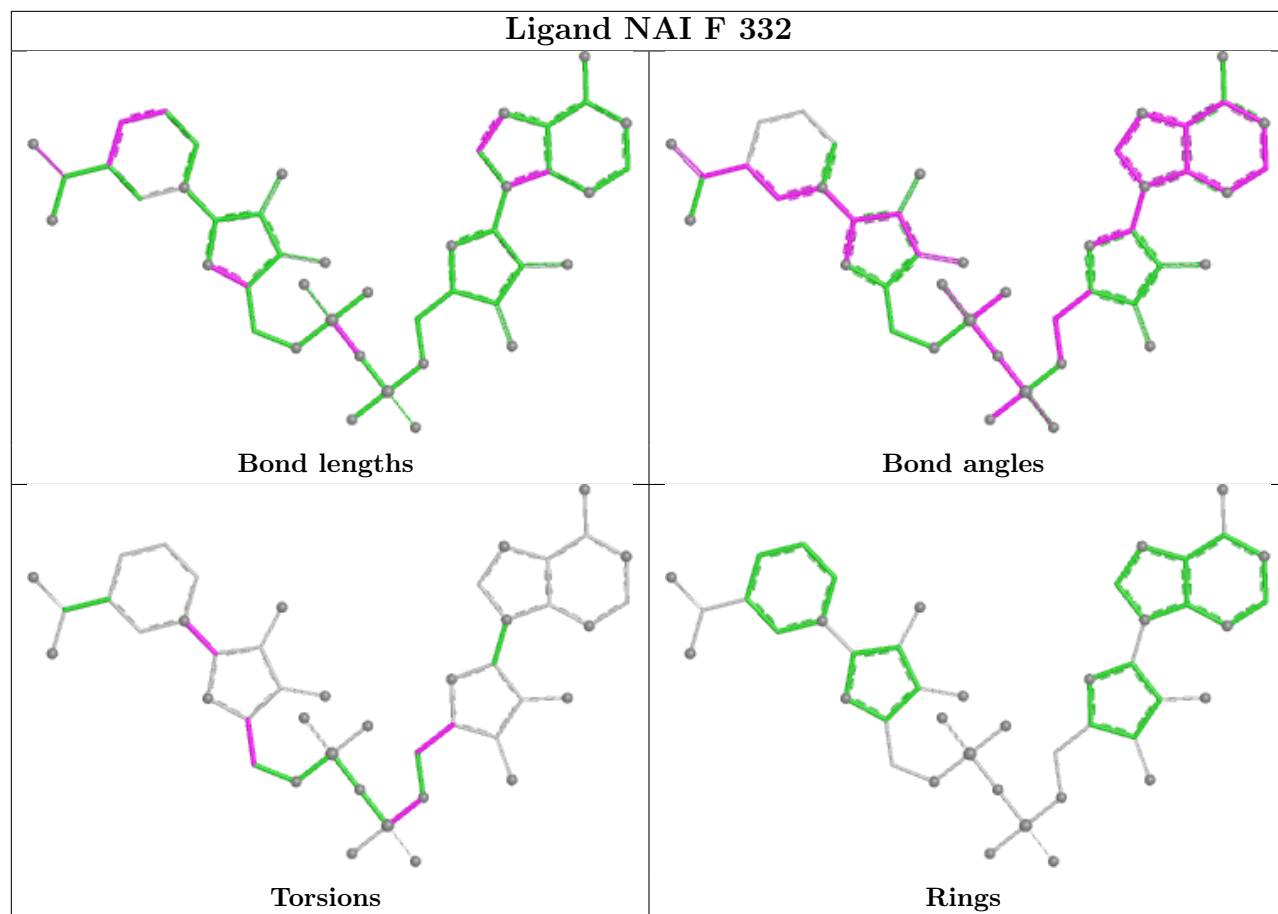
Ligand NAI A 332

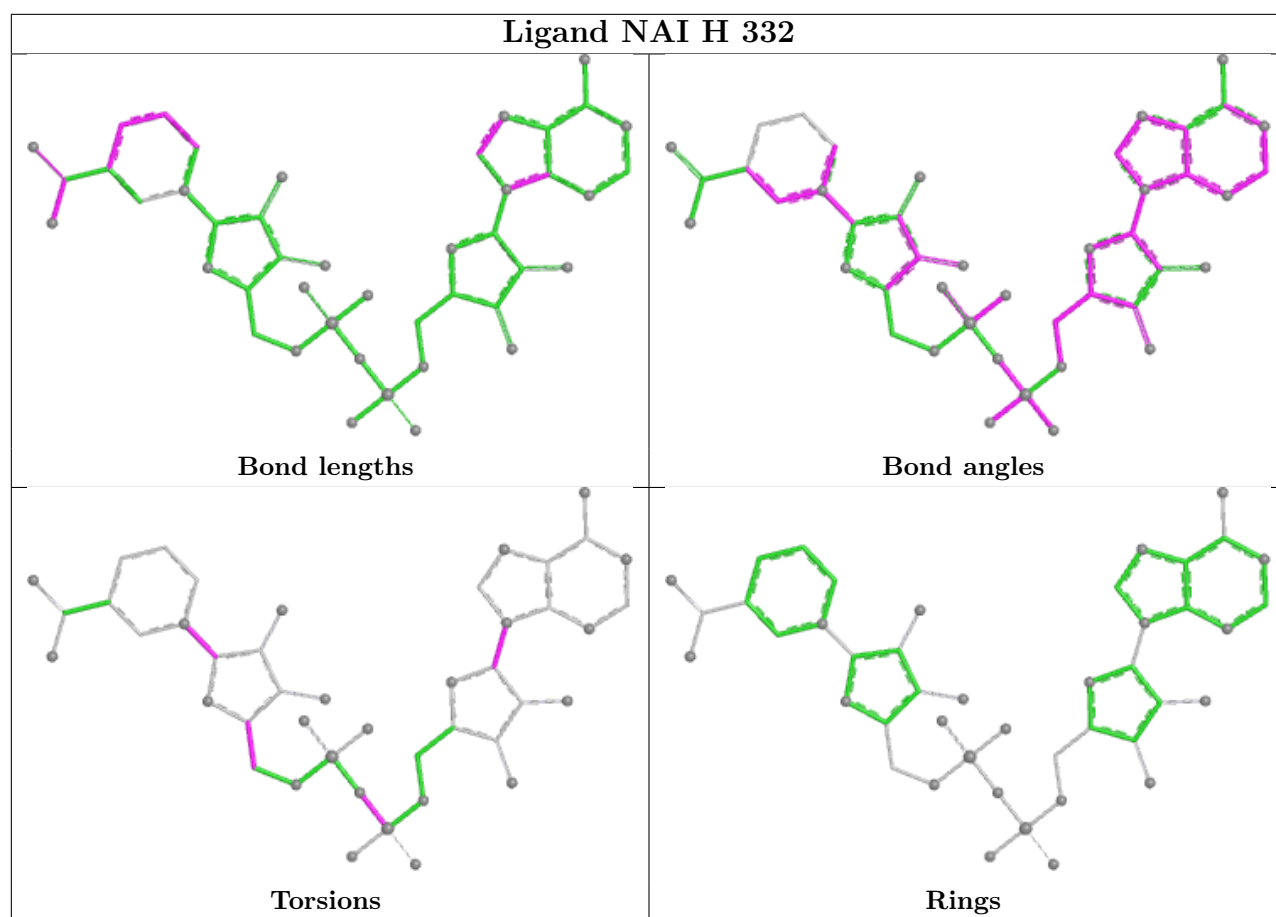


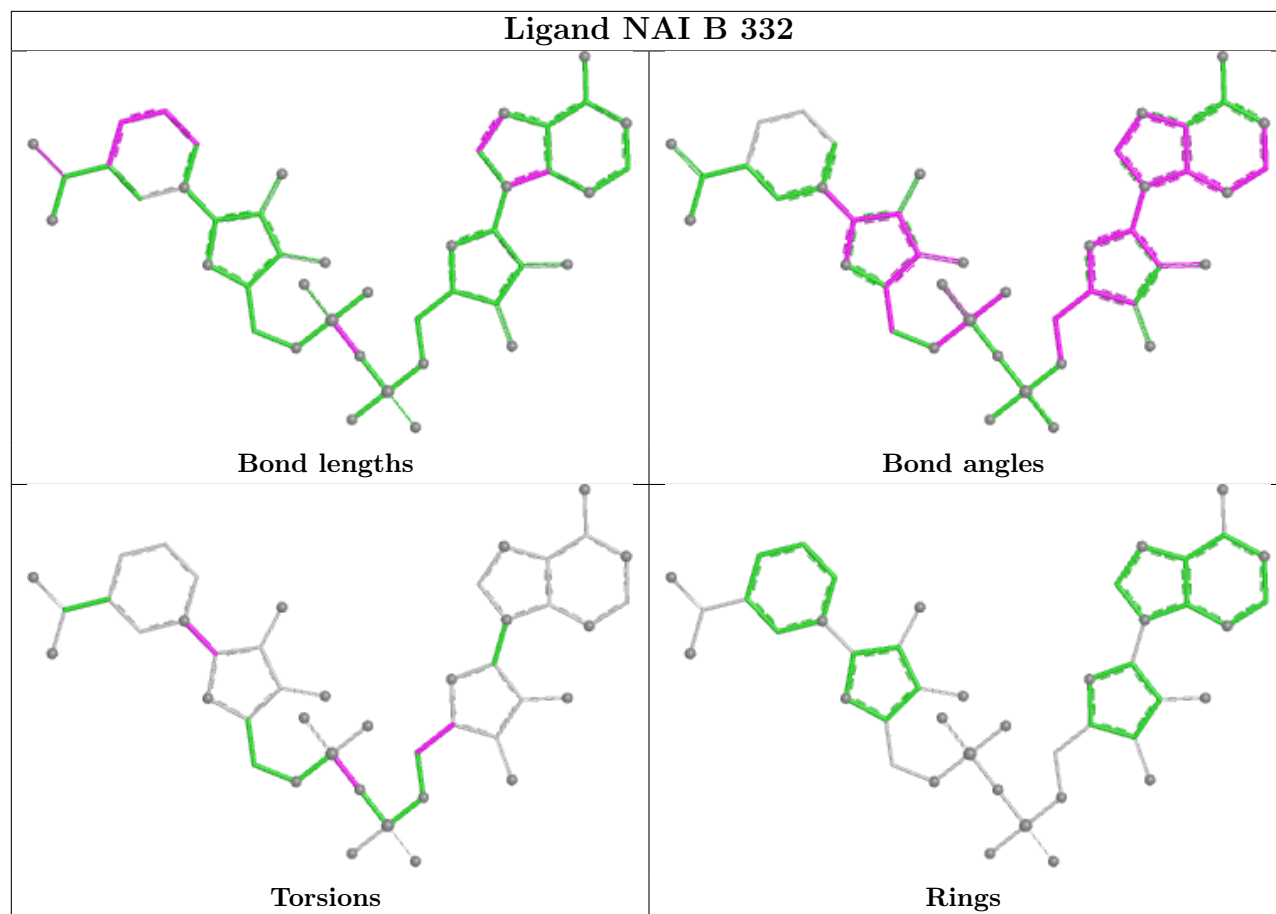
Ligand NAI D 332



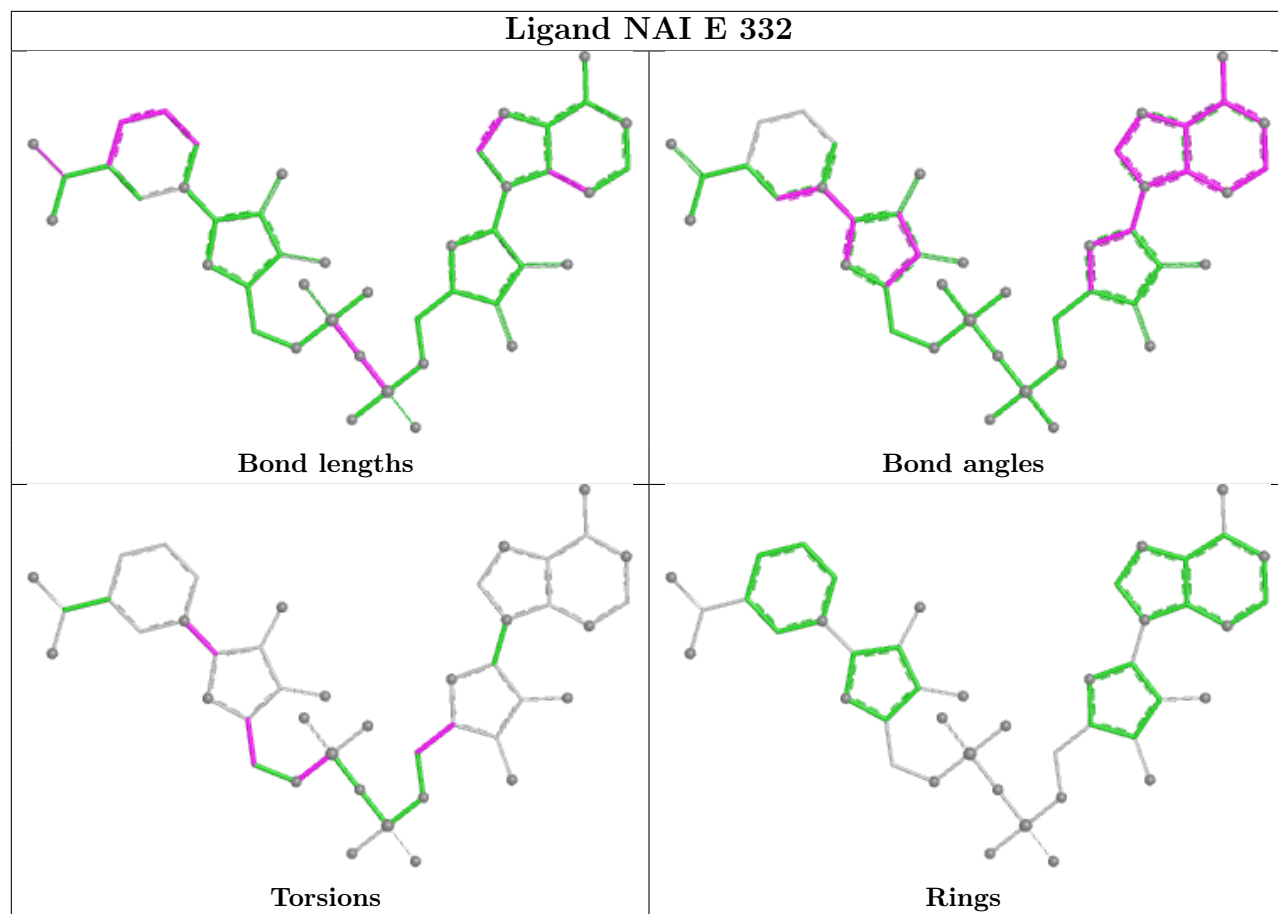
Ligand NAI F 332

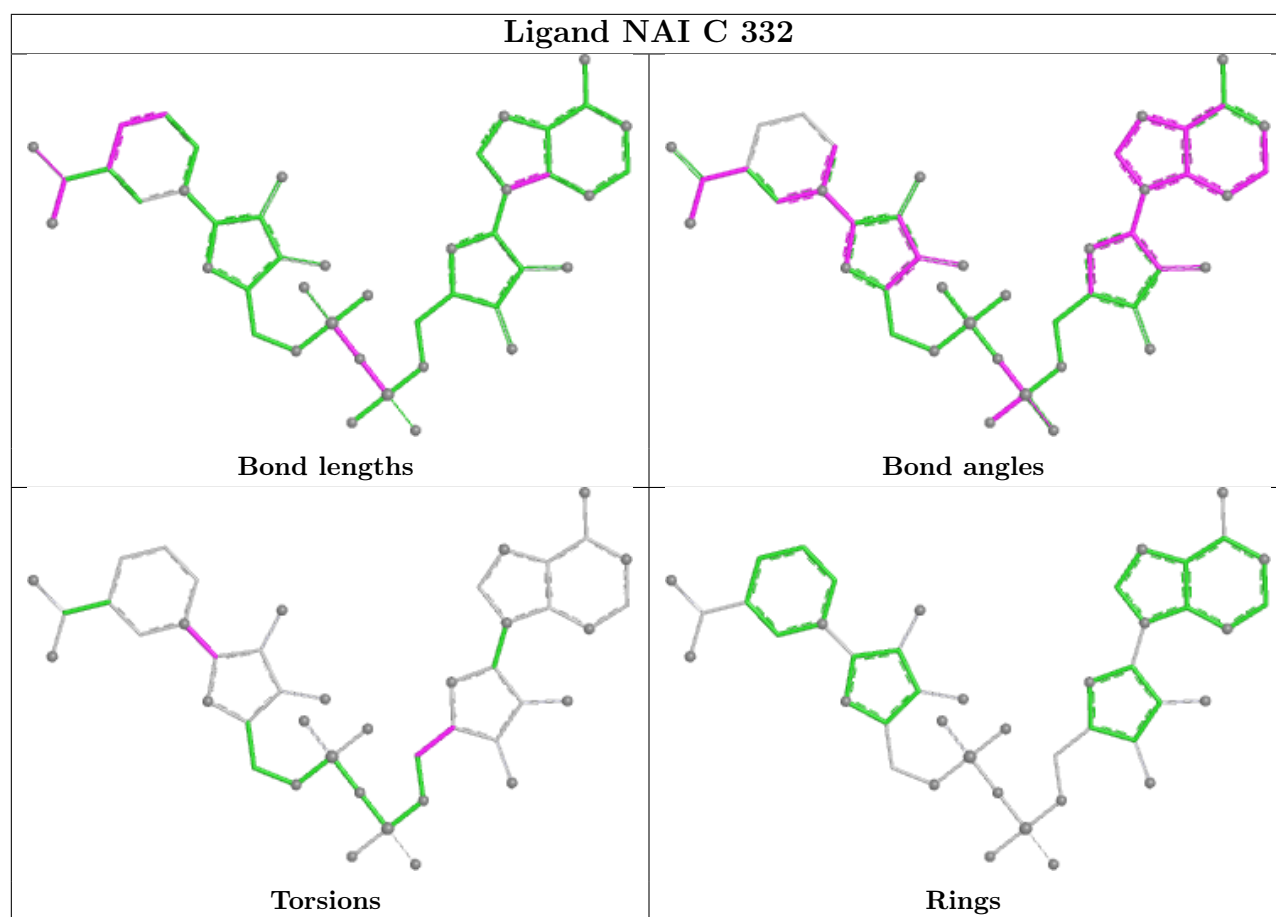






Ligand NAI E 332





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/331 (100%)	-0.54	1 (0%) 90 89	8, 18, 34, 52	1 (0%)
1	B	331/331 (100%)	-0.74	0 100 100	7, 16, 29, 43	2 (0%)
1	C	331/331 (100%)	-0.53	0 100 100	9, 18, 33, 46	0
1	D	331/331 (100%)	-0.51	0 100 100	8, 19, 33, 46	4 (1%)
1	E	331/331 (100%)	-0.35	2 (0%) 85 85	7, 20, 38, 53	1 (0%)
1	F	331/331 (100%)	-0.47	0 100 100	8, 17, 33, 43	1 (0%)
1	G	331/331 (100%)	-0.66	0 100 100	8, 19, 29, 43	3 (0%)
1	H	331/331 (100%)	-0.45	1 (0%) 90 89	7, 20, 35, 53	2 (0%)
All	All	2648/2648 (100%)	-0.53	4 (0%) 91 90	7, 19, 33, 53	14 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	GLY	2.4
1	E	331	PHE	2.2
1	E	2	ALA	2.2
1	H	100	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OXM	D	333	6/6	0.66	0.18	60,62,63,64	0
4	ACT	A	334	4/4	0.68	0.14	31,32,33,33	0
4	ACT	H	336	4/4	0.69	0.16	45,46,46,47	0
4	ACT	D	335	4/4	0.75	0.14	41,41,42,42	0
4	ACT	C	335	4/4	0.76	0.13	42,43,43,43	0
4	ACT	E	337	4/4	0.77	0.15	37,38,38,38	0
4	ACT	G	336	4/4	0.77	0.12	42,44,44,44	0
4	ACT	E	335	4/4	0.77	0.13	32,32,33,33	0
4	ACT	E	336	4/4	0.78	0.12	41,42,43,43	0
4	ACT	F	334	4/4	0.81	0.14	38,38,40,40	0
3	OXM	H	333	6/6	0.82	0.09	11,16,20,22	0
2	NAI	D	332	44/44	0.83	0.11	25,32,44,45	0
3	OXM	A	333	6/6	0.85	0.13	34,34,35,36	0
4	ACT	B	334	4/4	0.85	0.10	30,30,32,33	0
4	ACT	E	338	4/4	0.86	0.14	39,40,40,40	0
4	ACT	H	335	4/4	0.86	0.10	33,33,34,34	0
4	ACT	D	334	4/4	0.86	0.11	40,41,41,41	0
4	ACT	H	337	4/4	0.86	0.19	46,46,46,47	0
4	ACT	D	338	4/4	0.87	0.10	32,34,34,34	0
3	OXM	E	333	6/6	0.87	0.16	34,36,37,37	0
4	ACT	F	335	4/4	0.88	0.09	37,38,38,39	0
4	ACT	G	334	4/4	0.89	0.10	30,31,31,33	0
4	ACT	E	334	4/4	0.91	0.10	37,38,38,38	0
4	ACT	D	336	4/4	0.91	0.11	39,40,40,40	0
4	ACT	C	334	4/4	0.91	0.13	27,28,28,28	0
4	ACT	H	334	4/4	0.92	0.10	31,32,32,32	0
3	OXM	C	333	6/6	0.92	0.11	12,15,17,17	0
2	NAI	E	332	44/44	0.93	0.07	20,29,33,36	0
2	NAI	A	332	44/44	0.94	0.07	20,25,29,31	0
3	OXM	G	333	6/6	0.95	0.09	5,6,7,9	0
4	ACT	D	337	4/4	0.95	0.11	32,33,33,34	0
4	ACT	G	335	4/4	0.96	0.07	39,39,39,40	0
3	OXM	F	333	6/6	0.96	0.06	14,16,17,18	0
3	OXM	B	333	6/6	0.97	0.05	9,14,16,17	0
2	NAI	H	332	44/44	0.97	0.05	10,19,23,27	0
2	NAI	G	332	44/44	0.98	0.05	6,13,18,22	0
2	NAI	B	332	44/44	0.98	0.04	7,14,17,18	0

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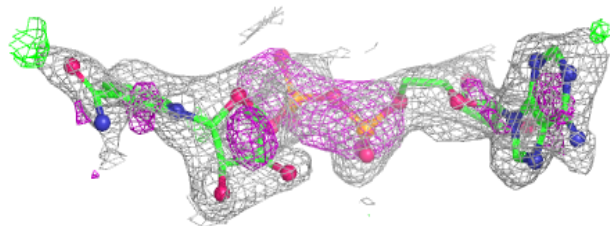
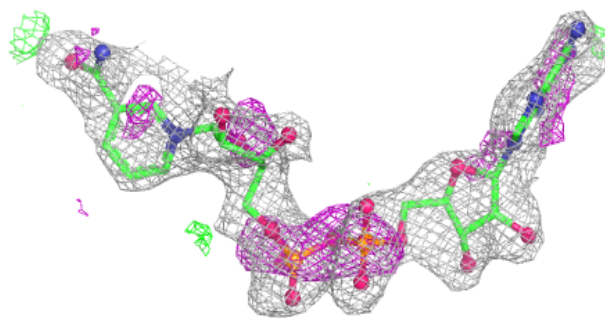
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAI	F	332	44/44	0.98	0.04	6,13,17,19	0
2	NAI	C	332	44/44	0.99	0.04	6,12,15,17	0

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

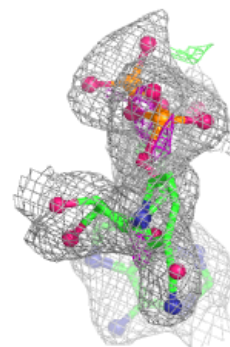
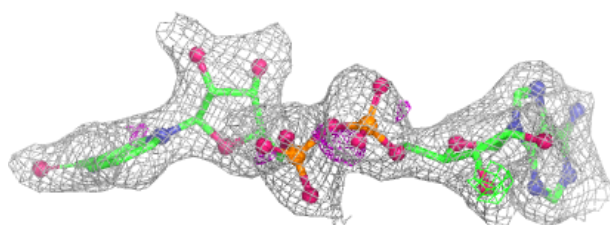
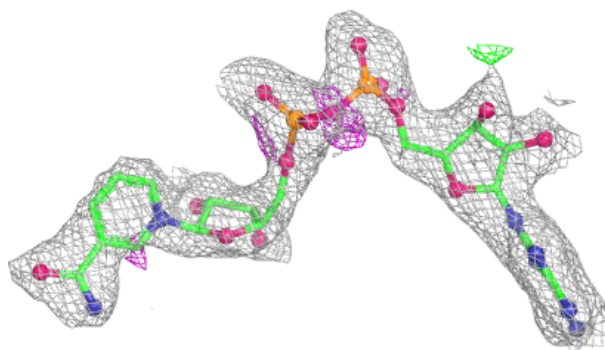
Electron density around NAI D 332:

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

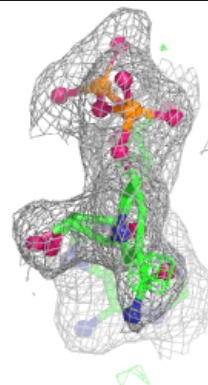
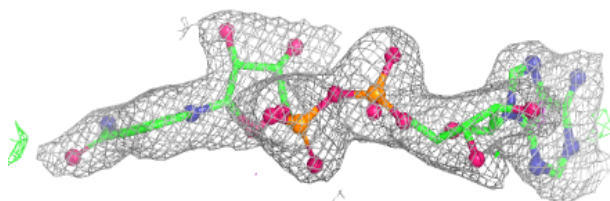
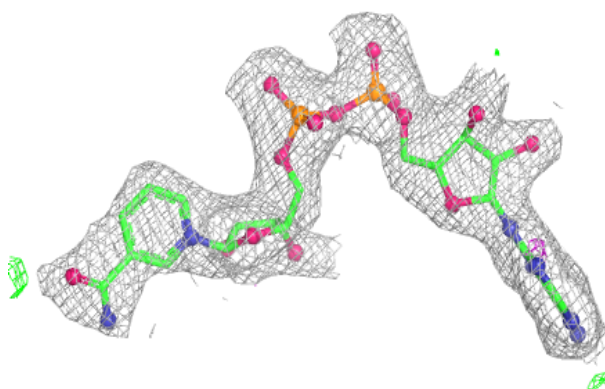


Electron density around NAI E 332:

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

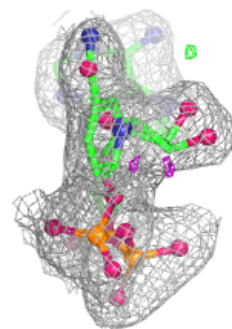
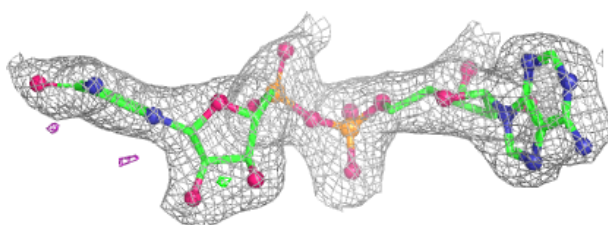
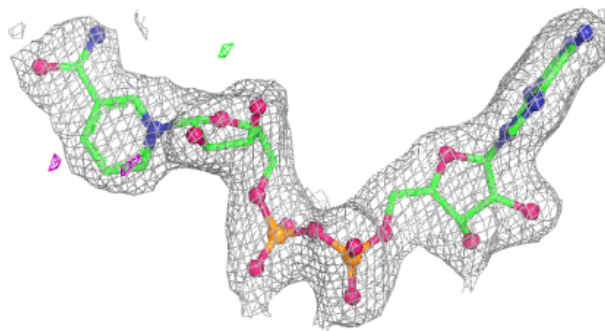
**Electron density around NAI A 332:**

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

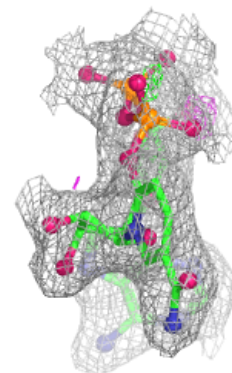
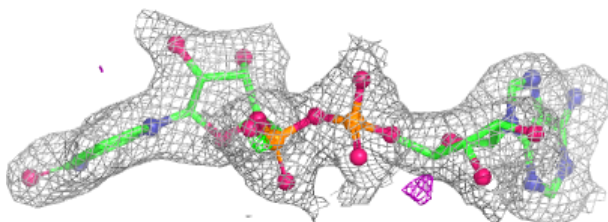
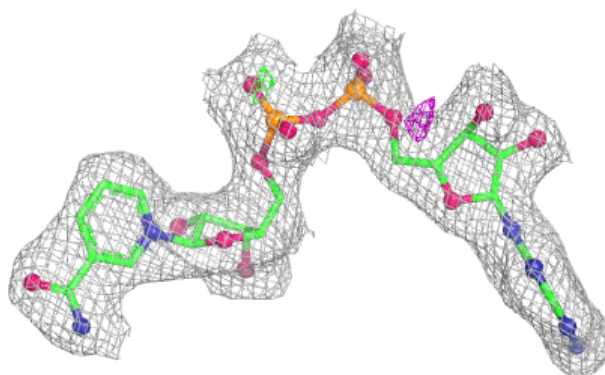


Electron density around NAI H 332:

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

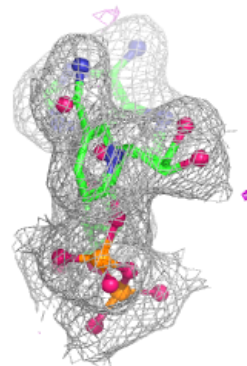
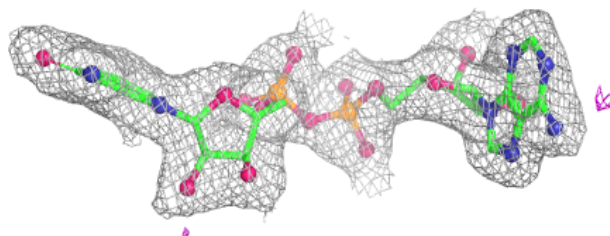
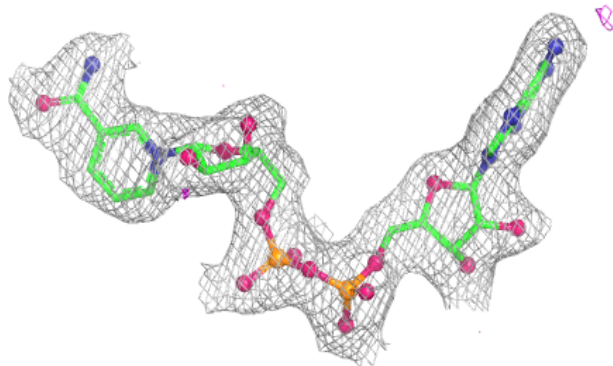
**Electron density around NAI G 332:**

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

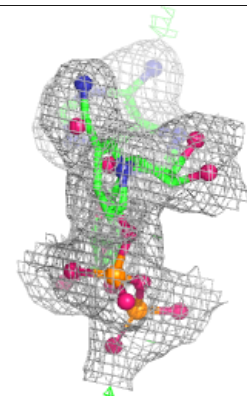
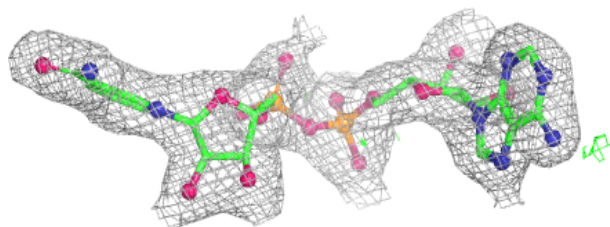
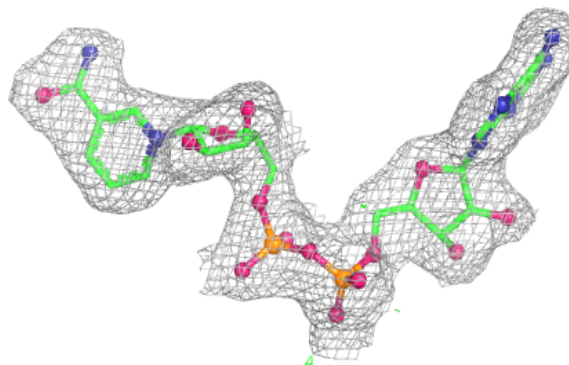


Electron density around NAI B 332:

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

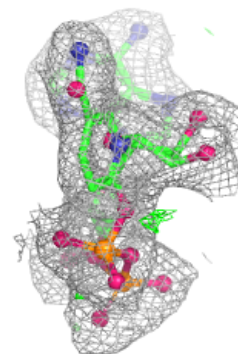
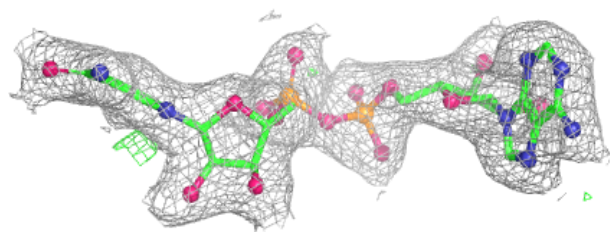
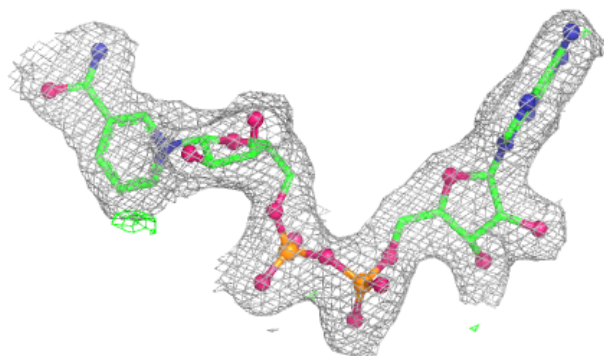
**Electron density around NAI F 332:**

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



Electron density around NAI C 332:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.