



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:18 AM UTC

PDB ID : 2DLD / pdb_00002dld
Title : D-LACTATE DEHYDROGENASE COMPLEXED WITH NADH AND OXAMATE
Authors : Dunn, C.R.; Holbrook, J.J.
Deposited on : 1995-10-28
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 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

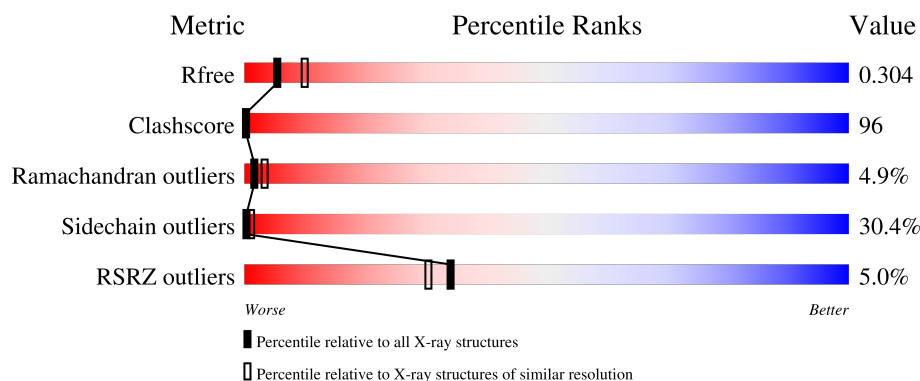
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	337	9% 17% 42% 34% 7%
1	B	337	% 18% 44% 28% 10%

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
2	NAI	A	401	X	-	-	-
2	NAI	B	401	-	-	X	-
3	OXM	A	402	-	-	X	-
3	OXM	B	402	-	X	X	-

2 Entry composition [i](#)

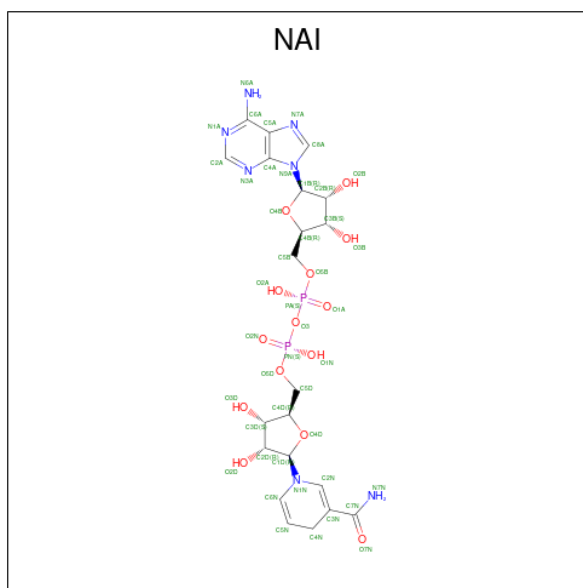
There are 3 unique types of molecules in this entry. The entry contains 5416 atoms, of which 0 are hydrogens and 0 are deuteriums.

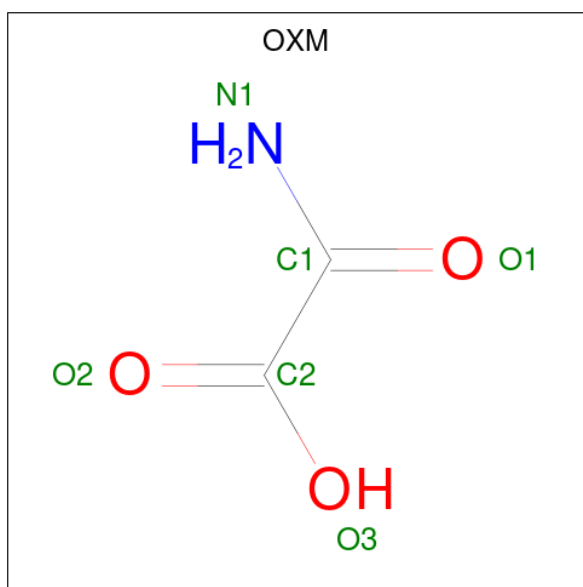
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called D-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2658	1684	458	504	12			
1	B	337	Total	C	N	O	S	0	0	0
			2658	1684	458	504	12			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



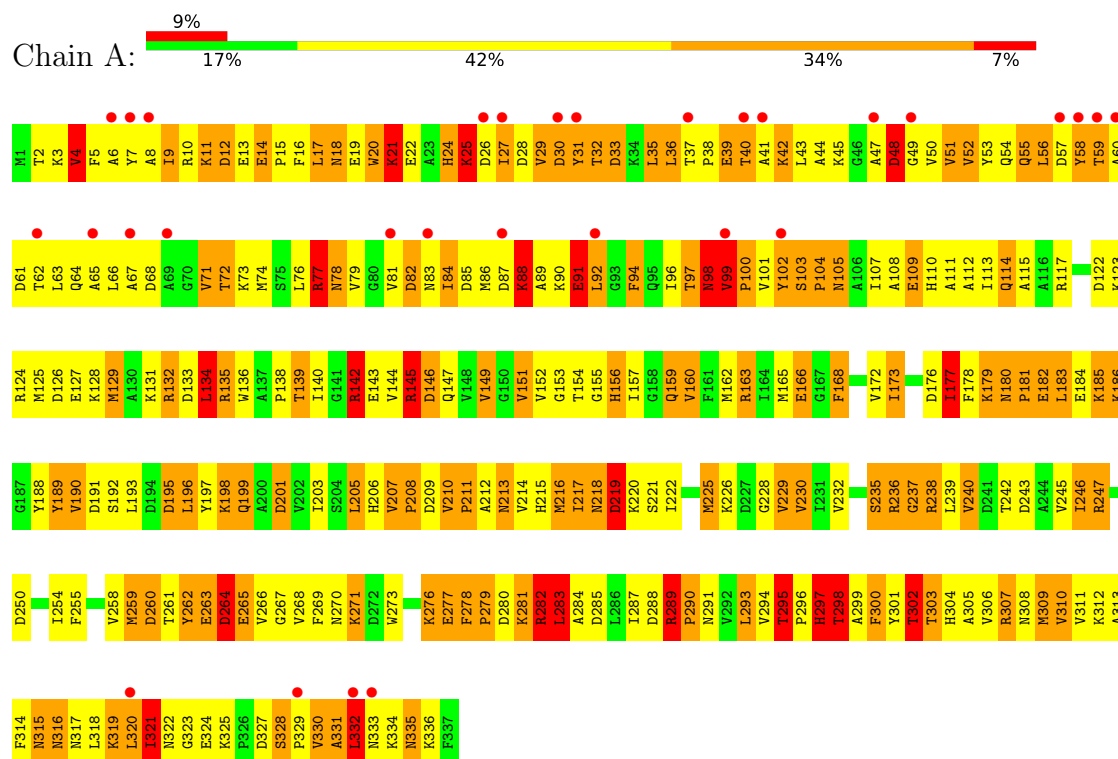


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	2	1	3		
3	B	1	Total	C	N	O	0	0
			6	2	1	3		

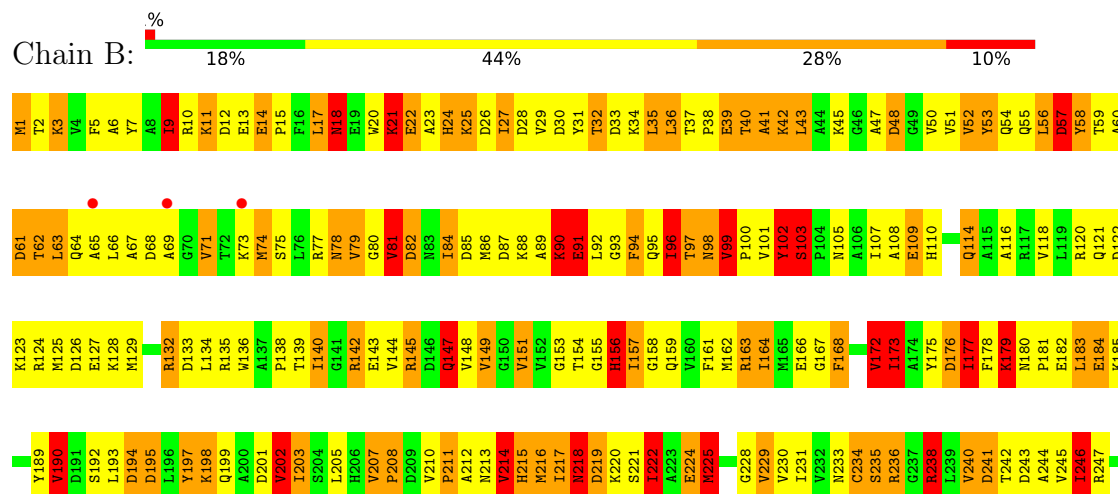
3 Residue-property plots

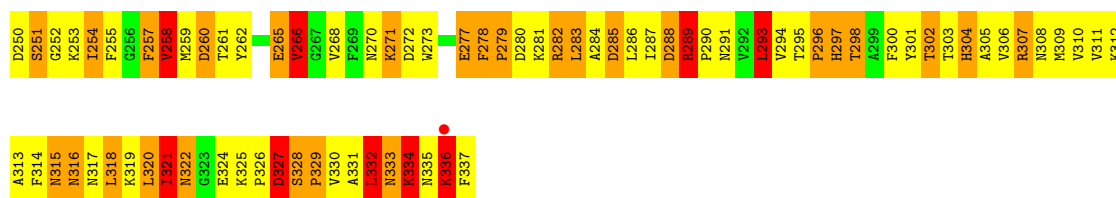
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: D-LACTATE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.20Å 62.10Å 77.40Å 90.00° 113.20° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 10.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	82.0 (10.00-2.70) 86.8 (10.00-2.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.71Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.195 , 0.297 0.211 , 0.304	Depositor DCC
R_{free} test set	1411 reflections (7.89%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5416	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, 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	1.32	7/2707 (0.3%)	2.17	132/3661 (3.6%)
1	B	1.36	7/2707 (0.3%)	2.19	129/3661 (3.5%)
All	All	1.34	14/5414 (0.3%)	2.18	261/7322 (3.6%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	ARG	CA-CB	-7.36	1.42	1.53
1	B	279	PRO	N-CA	-6.82	1.38	1.47
1	A	279	PRO	N-CA	-6.75	1.38	1.47
1	B	282	ARG	N-CA	6.61	1.54	1.46
1	B	148	VAL	C-N	-5.92	1.26	1.33
1	B	258	VAL	N-CA	5.87	1.53	1.46
1	A	127	GLU	CA-CB	-5.71	1.44	1.53
1	A	142	ARG	CD-NE	-5.55	1.38	1.46
1	A	25	LYS	N-CA	-5.39	1.39	1.46
1	A	207	VAL	N-CA	5.23	1.53	1.46
1	A	300	PHE	CA-CB	5.21	1.61	1.53
1	B	153	GLY	N-CA	5.15	1.52	1.45
1	B	236	ARG	N-CA	5.15	1.51	1.45
1	A	58	TYR	CA-C	5.13	1.58	1.53

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ASP	CA-CB-CG	19.50	132.10	112.60
1	A	289	ARG	CD-NE-CZ	14.03	144.04	124.40
1	B	288	ASP	CA-CB-CG	12.04	124.64	112.60
1	B	156	HIS	CA-CB-CG	12.01	125.81	113.80
1	B	304	HIS	CA-CB-CG	11.83	125.63	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	ASP	CA-CB-CG	11.21	123.81	112.60
1	A	146	ASP	CA-CB-CG	9.76	122.36	112.60
1	B	194	ASP	CA-CB-CG	9.66	122.26	112.60
1	A	111	ALA	CA-C-N	9.39	132.65	120.44
1	A	111	ALA	C-N-CA	9.39	132.65	120.44
1	B	218	ASN	CA-CB-CG	-9.39	103.21	112.60
1	A	98	ASN	CA-CB-CG	9.28	121.88	112.60
1	A	281	LYS	N-CA-C	9.16	121.03	111.14
1	A	195	ASP	CA-CB-CG	-9.15	103.45	112.60
1	B	142	ARG	CA-CB-CG	9.09	132.28	114.10
1	B	79	VAL	N-CA-C	8.96	118.84	110.42
1	B	157	ILE	N-CA-C	8.85	118.92	110.42
1	B	168	PHE	CA-CB-CG	-8.83	104.97	113.80
1	B	278	PHE	CA-C-N	8.81	129.69	119.47
1	B	278	PHE	C-N-CA	8.81	129.69	119.47
1	A	99	VAL	CA-C-N	8.73	128.95	119.87
1	A	99	VAL	C-N-CA	8.73	128.95	119.87
1	B	201	ASP	CA-CB-CG	8.72	121.32	112.60
1	A	149	VAL	CA-C-N	-8.50	114.83	122.73
1	A	149	VAL	C-N-CA	-8.50	114.83	122.73
1	A	279	PRO	N-CA-C	8.47	124.45	114.03
1	A	142	ARG	CD-NE-CZ	8.46	136.25	124.40
1	A	263	GLU	CA-CB-CG	8.39	130.88	114.10
1	A	24	HIS	CA-C-N	8.20	137.21	121.54
1	A	24	HIS	C-N-CA	8.20	137.21	121.54
1	B	53	TYR	CA-CB-CG	8.17	128.60	113.90
1	A	335	ASN	N-CA-C	-8.14	103.48	113.41
1	A	237	GLY	N-CA-C	8.00	122.59	112.83
1	B	234	CYS	CA-C-N	-7.96	111.04	121.79
1	B	234	CYS	C-N-CA	-7.96	111.04	121.79
1	A	278	PHE	CA-C-N	7.85	128.04	119.87
1	A	278	PHE	C-N-CA	7.85	128.04	119.87
1	A	264	ASP	CB-CA-C	7.82	123.13	111.17
1	B	148	VAL	N-CA-CB	7.70	121.16	111.46
1	A	203	ILE	CA-C-O	7.68	127.83	120.31
1	A	105	ASN	CA-CB-CG	-7.66	104.94	112.60
1	B	207	VAL	N-CA-CB	-7.45	103.67	111.87
1	B	18	ASN	CA-CB-CG	-7.41	105.19	112.60
1	A	262	TYR	CA-CB-CG	7.41	127.23	113.90
1	B	14	GLU	CA-C-N	7.38	128.03	119.47
1	B	14	GLU	C-N-CA	7.38	128.03	119.47
1	A	126	ASP	CA-CB-CG	7.38	119.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ARG	N-CA-C	-7.34	104.35	113.38
1	B	278	PHE	CA-C-O	7.32	125.09	119.46
1	B	172	VAL	CA-C-N	7.28	132.49	123.10
1	B	172	VAL	C-N-CA	7.28	132.49	123.10
1	B	327	ASP	CA-CB-CG	-7.27	105.33	112.60
1	B	229	VAL	O-C-N	7.24	130.00	122.54
1	A	18	ASN	CA-CB-CG	7.21	119.81	112.60
1	B	81	VAL	CB-CA-C	-7.19	102.51	112.36
1	A	207	VAL	N-CA-CB	-7.16	101.19	111.21
1	B	258	VAL	CA-C-O	-7.12	112.82	120.36
1	A	91	GLU	N-CA-C	-7.09	102.67	111.75
1	B	265	GLU	CB-CG-CD	7.05	124.58	112.60
1	B	293	LEU	N-CA-CB	7.03	122.33	110.87
1	B	285	ASP	CA-C-O	7.01	128.20	120.63
1	A	114	GLN	OE1-CD-NE2	-7.00	115.60	122.60
1	A	218	ASN	CA-CB-CG	-6.99	105.61	112.60
1	A	283	LEU	N-CA-C	-6.99	103.67	111.28
1	A	122	ASP	CA-CB-CG	-6.93	105.67	112.60
1	A	282	ARG	NE-CZ-NH1	-6.93	114.57	121.50
1	A	180	ASN	CA-CB-CG	6.91	119.51	112.60
1	B	216	MET	CA-C-N	-6.88	114.41	122.95
1	B	216	MET	C-N-CA	-6.88	114.41	122.95
1	A	48	ASP	N-CA-C	6.87	119.41	111.02
1	B	282	ARG	N-CA-C	-6.87	103.72	111.14
1	B	144	VAL	CB-CA-C	-6.84	102.91	112.14
1	A	55	GLN	N-CA-C	-6.82	104.99	113.38
1	B	218	ASN	OD1-CG-ND2	6.81	129.41	122.60
1	B	99	VAL	CA-C-N	6.81	126.27	118.85
1	B	99	VAL	C-N-CA	6.81	126.27	118.85
1	A	336	LYS	CA-C-N	6.78	133.90	121.70
1	A	336	LYS	C-N-CA	6.78	133.90	121.70
1	A	293	LEU	CA-CB-CG	6.75	139.92	116.30
1	B	253	LYS	N-CA-C	-6.72	103.95	111.28
1	B	139	THR	CA-CB-OG1	-6.61	99.68	109.60
1	B	235	SER	CA-C-O	6.61	123.53	119.77
1	A	78	ASN	CA-C-N	6.57	130.86	120.47
1	A	78	ASN	C-N-CA	6.57	130.86	120.47
1	A	57	ASP	N-CA-C	6.56	119.80	109.96
1	A	235	SER	CA-C-O	6.53	123.53	119.55
1	A	282	ARG	CD-NE-CZ	-6.46	115.36	124.40
1	A	278	PHE	CA-CB-CG	-6.44	107.36	113.80
1	B	266	VAL	N-CA-CB	6.41	118.72	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	LYS	N-CA-C	-6.38	105.22	112.87
1	A	298	THR	CB-CA-C	6.36	120.06	109.38
1	B	190	VAL	CA-C-O	-6.31	113.96	121.28
1	A	115	ALA	O-C-N	6.29	128.57	122.03
1	A	112	ALA	O-C-N	6.26	128.52	122.07
1	A	276	LYS	CA-C-N	-6.25	114.11	122.42
1	A	276	LYS	C-N-CA	-6.25	114.11	122.42
1	B	336	LYS	CA-C-N	6.24	132.94	121.70
1	B	336	LYS	C-N-CA	6.24	132.94	121.70
1	B	9	ILE	N-CA-C	6.24	116.48	108.12
1	B	293	LEU	CA-C-N	-6.23	114.01	122.91
1	B	293	LEU	C-N-CA	-6.23	114.01	122.91
1	A	203	ILE	CA-C-N	-6.22	114.28	123.11
1	A	203	ILE	C-N-CA	-6.22	114.28	123.11
1	B	100	PRO	N-CA-C	6.20	121.71	113.40
1	B	257	PHE	CA-C-O	-6.20	113.86	121.11
1	A	100	PRO	N-CA-C	6.17	121.62	114.03
1	B	236	ARG	CB-CA-C	6.16	119.97	109.80
1	A	26	ASP	CA-CB-CG	6.13	118.73	112.60
1	B	238	ARG	CA-C-N	6.13	129.11	120.28
1	B	238	ARG	C-N-CA	6.13	129.11	120.28
1	A	315	ASN	CA-CB-CG	-6.09	106.51	112.60
1	A	300	PHE	CA-C-N	6.08	133.15	121.54
1	A	300	PHE	C-N-CA	6.08	133.15	121.54
1	A	160	VAL	O-C-N	6.07	127.86	121.91
1	B	173	ILE	CB-CA-C	-6.07	101.58	110.81
1	A	42	LYS	N-CA-C	6.05	118.67	111.71
1	A	41	ALA	CA-C-N	6.05	128.99	120.28
1	A	41	ALA	C-N-CA	6.05	128.99	120.28
1	B	303	THR	N-CA-CB	-6.04	101.00	110.06
1	A	260	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	202	VAL	CA-C-O	-6.03	113.84	120.72
1	B	254	ILE	N-CA-C	6.03	116.98	108.36
1	B	105	ASN	OD1-CG-ND2	6.02	128.62	122.60
1	A	213	ASN	CA-CB-CG	-6.02	106.58	112.60
1	A	302	THR	N-CA-C	6.01	118.42	108.99
1	A	14	GLU	CA-C-N	6.00	125.71	119.05
1	A	14	GLU	C-N-CA	6.00	125.71	119.05
1	B	327	ASP	N-CA-C	5.97	118.46	108.96
1	B	136	TRP	N-CA-C	5.97	118.68	111.40
1	A	247	ARG	CA-C-N	5.96	127.78	120.22
1	A	247	ARG	C-N-CA	5.96	127.78	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	HIS	CA-C-N	-5.95	112.89	122.23
1	A	297	HIS	C-N-CA	-5.95	112.89	122.23
1	B	78	ASN	CA-CB-CG	-5.93	106.67	112.60
1	B	51	VAL	CA-C-N	-5.90	111.35	121.97
1	B	51	VAL	C-N-CA	-5.90	111.35	121.97
1	B	109	GLU	CB-CG-CD	5.89	122.61	112.60
1	A	29	VAL	N-CA-C	5.88	116.59	108.12
1	A	195	ASP	O-C-N	5.86	128.91	122.11
1	B	103	SER	CA-C-N	5.85	125.47	119.56
1	B	103	SER	C-N-CA	5.85	125.47	119.56
1	B	102	TYR	CB-CA-C	-5.85	103.73	112.09
1	B	166	GLU	N-CA-C	-5.84	104.87	112.23
1	B	102	TYR	CA-CB-CG	5.84	124.40	113.90
1	B	224	GLU	O-C-N	5.83	128.29	122.12
1	A	307	ARG	N-CA-C	-5.79	104.87	111.07
1	B	257	PHE	N-CA-CB	-5.76	100.88	111.37
1	B	91	GLU	N-CA-C	-5.75	104.38	111.33
1	B	57	ASP	CA-CB-CG	-5.72	106.88	112.60
1	B	96	ILE	CA-C-O	5.71	127.67	121.67
1	B	59	THR	CA-C-N	5.71	132.44	121.54
1	B	59	THR	C-N-CA	5.71	132.44	121.54
1	B	58	TYR	N-CA-C	-5.70	101.06	109.62
1	A	112	ALA	CB-CA-C	-5.70	101.93	110.88
1	A	72	THR	N-CA-C	-5.69	105.07	113.61
1	B	26	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	190	VAL	N-CA-C	-5.67	99.62	108.86
1	B	163	ARG	CD-NE-CZ	5.67	132.34	124.40
1	B	25	LYS	N-CA-C	5.66	118.18	111.33
1	A	78	ASN	CA-CB-CG	5.65	118.25	112.60
1	B	300	PHE	CA-CB-CG	-5.64	108.16	113.80
1	B	203	ILE	CA-C-N	-5.63	114.85	123.07
1	B	203	ILE	C-N-CA	-5.63	114.85	123.07
1	A	58	TYR	N-CA-CB	5.62	116.64	110.35
1	A	211	PRO	N-CA-C	-5.61	105.40	113.75
1	B	296	PRO	N-CA-CB	5.60	106.82	102.73
1	A	203	ILE	O-C-N	-5.59	117.61	123.03
1	A	216	MET	CA-C-N	-5.58	115.62	122.93
1	A	216	MET	C-N-CA	-5.58	115.62	122.93
1	B	167	GLY	N-CA-C	-5.58	106.03	112.50
1	B	201	ASP	CA-C-O	5.58	126.08	119.67
1	B	195	ASP	CA-C-O	5.57	126.51	120.55
1	A	180	ASN	CA-C-N	5.57	126.80	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASN	C-N-CA	5.57	126.80	119.84
1	A	321	ILE	CA-C-N	5.56	131.44	121.66
1	A	321	ILE	C-N-CA	5.56	131.44	121.66
1	A	21	LYS	N-CA-C	-5.54	104.87	111.69
1	A	243	ASP	CA-C-N	5.54	128.16	120.63
1	A	243	ASP	C-N-CA	5.54	128.16	120.63
1	A	230	VAL	CA-C-N	-5.53	115.89	123.14
1	A	230	VAL	C-N-CA	-5.53	115.89	123.14
1	A	230	VAL	CA-C-O	-5.53	114.50	120.36
1	B	296	PRO	CA-C-O	-5.53	115.44	123.07
1	B	176	ASP	N-CA-C	5.52	117.50	108.55
1	A	208	PRO	N-CA-CB	5.51	108.57	103.39
1	A	279	PRO	N-CA-CB	5.51	108.59	103.41
1	A	177	ILE	N-CA-C	-5.51	105.36	110.53
1	B	164	ILE	CB-CA-C	-5.49	104.95	111.97
1	A	265	GLU	CA-CB-CG	5.47	125.04	114.10
1	B	329	PRO	N-CA-CB	5.47	108.11	103.19
1	A	295	THR	N-CA-CB	5.46	121.02	111.19
1	A	88	LYS	CA-C-N	5.44	127.57	120.28
1	A	88	LYS	C-N-CA	5.44	127.57	120.28
1	A	55	GLN	N-CA-CB	5.43	118.63	110.53
1	B	289	ARG	CA-C-N	5.43	126.63	119.84
1	B	289	ARG	C-N-CA	5.43	126.63	119.84
1	A	129	MET	N-CA-CB	5.43	117.94	110.07
1	B	266	VAL	O-C-N	5.43	128.21	122.67
1	A	316	ASN	CA-CB-CG	-5.41	107.19	112.60
1	B	139	THR	N-CA-CB	-5.40	101.37	110.49
1	B	96	ILE	N-CA-C	5.39	117.85	108.95
1	B	222	ILE	CB-CG1-CD1	-5.39	102.48	113.80
1	B	245	VAL	N-CA-CB	5.38	116.48	110.51
1	B	208	PRO	CA-C-N	5.37	131.80	121.54
1	B	208	PRO	C-N-CA	5.37	131.80	121.54
1	A	199	GLN	CA-C-O	5.37	124.42	118.52
1	B	240	VAL	CB-CA-C	-5.37	103.87	111.38
1	A	265	GLU	CB-CG-CD	5.35	121.69	112.60
1	A	300	PHE	N-CA-C	5.34	119.90	112.90
1	B	127	GLU	CA-CB-CG	5.34	124.78	114.10
1	B	260	ASP	N-CA-C	-5.33	106.72	114.12
1	A	207	VAL	CB-CA-C	5.32	121.04	111.36
1	B	149	VAL	N-CA-CB	-5.32	104.76	111.46
1	B	148	VAL	CB-CA-C	-5.31	103.21	110.96
1	A	291	ASN	O-C-N	5.30	129.12	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	PRO	N-CA-C	5.30	121.49	113.81
1	A	168	PHE	N-CA-C	-5.29	106.78	113.18
1	A	199	GLN	N-CA-C	-5.25	106.39	114.16
1	B	260	ASP	CA-C-O	5.25	124.67	118.90
1	B	322	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	300	PHE	CA-CB-CG	-5.24	108.56	113.80
1	B	173	ILE	CA-C-O	-5.22	114.76	120.72
1	B	218	ASN	CA-C-O	-5.22	115.15	121.32
1	A	201	ASP	N-CA-C	-5.22	107.04	113.41
1	A	71	VAL	N-CA-C	5.20	116.15	108.45
1	A	201	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	283	LEU	N-CA-CB	5.17	118.21	109.78
1	A	134	LEU	CA-C-O	-5.15	113.14	120.51
1	A	124	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	B	90	LYS	CA-C-N	-5.14	113.34	120.38
1	B	90	LYS	C-N-CA	-5.14	113.34	120.38
1	A	129	MET	CA-CB-CG	5.12	124.33	114.10
1	B	147	GLN	CA-CB-CG	-5.11	103.88	114.10
1	A	4	VAL	CA-C-O	-5.10	114.95	120.36
1	A	290	PRO	CA-C-N	-5.10	114.48	122.49
1	A	290	PRO	C-N-CA	-5.10	114.48	122.49
1	B	321	ILE	CB-CA-C	-5.10	105.45	111.97
1	B	250	ASP	CA-C-N	5.09	127.52	120.29
1	B	250	ASP	C-N-CA	5.09	127.52	120.29
1	A	142	ARG	NH1-CZ-NH2	-5.09	112.69	119.30
1	B	153	GLY	CA-C-O	-5.09	111.72	120.57
1	B	246	ILE	CA-C-O	5.09	126.24	120.95
1	A	236	ARG	CA-C-N	5.08	125.72	120.03
1	A	236	ARG	C-N-CA	5.08	125.72	120.03
1	B	21	LYS	N-CA-C	-5.08	105.64	111.07
1	B	251	SER	CA-C-O	5.07	125.80	120.42
1	A	72	THR	N-CA-CB	5.06	118.34	110.80
1	B	114	GLN	CA-C-N	5.06	127.32	120.44
1	B	114	GLN	C-N-CA	5.06	127.32	120.44
1	A	213	ASN	N-CA-C	5.06	119.08	113.01
1	A	83	ASN	CA-CB-CG	5.05	117.65	112.60
1	B	214	VAL	N-CA-C	5.05	119.84	109.34
1	A	104	PRO	N-CA-C	-5.05	107.82	114.03
1	A	281	LYS	CA-CB-CG	-5.04	104.02	114.10
1	A	189	TYR	CA-C-O	5.04	126.81	121.16
1	B	79	VAL	CA-C-N	5.03	131.27	121.41
1	B	79	VAL	C-N-CA	5.03	131.27	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	VAL	CA-C-N	5.03	131.14	121.54
1	B	214	VAL	C-N-CA	5.03	131.14	121.54
1	A	159	GLN	CA-C-O	5.00	125.80	120.24
1	A	304	HIS	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2658	0	2661	541	0
1	B	2658	0	2661	523	0
2	A	44	0	24	16	0
2	B	44	0	25	28	0
3	A	6	0	2	4	0
3	B	6	0	2	11	0
All	All	5416	0	5375	1036	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 96.

All (1036) 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)
2:B:401:NAI:H5N	3:B:402:OXM:N1	1.31	1.44
1:A:53:TYR:CE1	1:A:78:ASN:HB3	1.54	1.40
1:A:25:LYS:HZ3	1:A:25:LYS:CA	1.44	1.29
1:B:86:MET:CE	1:B:332:LEU:HA	1.67	1.24
1:A:85:ASP:OD2	1:A:88:LYS:HB2	1.37	1.24
1:A:96:ILE:CG2	1:A:330:VAL:HG21	1.69	1.21
1:A:53:TYR:CE1	1:A:78:ASN:CB	2.26	1.18
1:B:81:VAL:HG12	1:B:84:ILE:HD11	1.25	1.18
1:B:162:MET:HE2	1:B:172:VAL:HG11	1.24	1.16
1:A:149:VAL:HG21	1:A:165:MET:HE3	1.26	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HG22	1:A:330:VAL:CG2	1.76	1.15
1:A:157:ILE:HD12	2:A:401:NAI:H51N	1.28	1.15
1:A:3:LYS:HB3	1:A:47:ALA:HA	1.29	1.14
1:B:48:ASP:OD1	1:B:73:LYS:NZ	1.80	1.14
1:A:19:GLU:HA	1:A:22:GLU:OE1	1.48	1.13
1:B:81:VAL:HG11	1:B:330:VAL:HG11	1.28	1.13
1:A:3:LYS:HG2	1:A:47:ALA:CB	1.77	1.13
1:A:3:LYS:HG2	1:A:47:ALA:HB1	1.26	1.12
1:B:162:MET:HE2	1:B:172:VAL:CG1	1.77	1.12
1:A:25:LYS:CA	1:A:25:LYS:NZ	2.12	1.12
1:A:38:PRO:HA	1:A:62:THR:HG23	1.26	1.11
1:B:85:ASP:OD2	1:B:88:LYS:HB2	1.51	1.11
1:B:316:ASN:ND2	1:B:327:ASP:O	1.85	1.10
1:A:306:VAL:HA	1:A:309:MET:HG3	1.14	1.10
1:B:86:MET:HE2	1:B:332:LEU:HA	1.27	1.10
1:A:96:ILE:HG22	1:A:330:VAL:HG21	1.09	1.09
1:A:3:LYS:HD3	1:A:47:ALA:HB2	1.35	1.08
1:A:9:ILE:HD12	1:A:77:ARG:NH1	1.69	1.07
1:A:21:LYS:HE2	1:A:21:LYS:HA	1.09	1.07
1:B:90:LYS:HB2	1:B:332:LEU:HD12	1.36	1.07
1:B:222:ILE:O	1:B:225:MET:HB2	1.54	1.06
1:B:74:MET:O	1:B:96:ILE:HG23	1.55	1.06
1:A:84:ILE:CD1	1:A:86:MET:SD	2.44	1.04
1:A:245:VAL:HG13	1:A:254:ILE:CD1	1.87	1.04
1:B:66:LEU:HD23	1:B:94:PHE:HZ	1.22	1.04
2:B:401:NAI:C5N	3:B:402:OXM:C1	2.35	1.04
1:A:7:TYR:HB2	1:A:52:VAL:HB	1.04	1.03
1:A:25:LYS:NZ	1:A:25:LYS:HA	1.72	1.03
1:B:1:MET:HG3	1:B:2:THR:N	1.66	1.03
1:A:176:ASP:OD1	2:A:401:NAI:N3A	1.92	1.03
1:A:277:GLU:HA	1:A:277:GLU:OE1	1.51	1.03
1:A:310:VAL:O	1:A:313:ALA:HB3	1.57	1.03
1:B:218:ASN:ND2	1:B:220:LYS:H	1.56	1.03
1:A:5:PHE:O	1:A:50:VAL:HG13	1.59	1.02
1:B:218:ASN:HD22	1:B:219:ASP:N	1.56	1.02
1:B:2:THR:HB	1:B:27:ILE:HG23	1.38	1.02
1:B:332:LEU:HD23	1:B:332:LEU:C	1.86	1.00
1:B:36:LEU:HD12	1:B:37:THR:N	1.76	1.00
1:B:18:ASN:N	1:B:18:ASN:HD22	1.45	1.00
1:A:84:ILE:HD13	1:A:86:MET:SD	2.02	1.00
1:B:54:GLN:NE2	1:B:56:LEU:HB3	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:HD12	2:B:401:NAI:H51N	1.44	0.99
1:A:38:PRO:CA	1:A:62:THR:HG23	1.93	0.99
1:A:21:LYS:HE2	1:A:21:LYS:CA	1.88	0.99
1:A:270:ASN:O	1:A:270:ASN:OD1	1.79	0.99
1:A:210:VAL:HG22	1:A:211:PRO:HD2	1.43	0.98
1:B:63:LEU:N	1:B:63:LEU:HD12	1.75	0.98
1:B:21:LYS:CA	1:B:21:LYS:HE2	1.92	0.98
1:B:35:LEU:HD23	1:B:35:LEU:N	1.75	0.98
1:A:25:LYS:HZ3	1:A:25:LYS:HA	0.84	0.97
1:B:66:LEU:HD23	1:B:94:PHE:CZ	1.99	0.97
1:A:18:ASN:O	1:A:22:GLU:N	1.98	0.96
1:A:190:VAL:HG11	1:A:195:ASP:HB2	1.45	0.96
1:B:18:ASN:N	1:B:18:ASN:ND2	2.09	0.96
1:A:2:THR:HB	1:A:27:ILE:HG23	1.47	0.96
1:B:54:GLN:NE2	1:B:56:LEU:O	1.97	0.96
1:A:7:TYR:CB	1:A:52:VAL:HB	1.95	0.96
1:A:7:TYR:HB2	1:A:52:VAL:CB	1.95	0.95
1:B:81:VAL:CG1	1:B:84:ILE:HD11	1.97	0.95
1:B:154:THR:HG22	1:B:154:THR:O	1.66	0.95
1:A:53:TYR:CD1	1:A:78:ASN:HB3	2.02	0.95
1:B:177:ILE:HG22	1:B:178:PHE:N	1.79	0.95
1:B:218:ASN:HD22	1:B:218:ASN:C	1.75	0.94
1:A:9:ILE:HG21	1:A:31:TYR:CD2	2.03	0.94
1:A:245:VAL:HG13	1:A:254:ILE:HD12	1.47	0.94
1:A:210:VAL:HG13	1:A:212:ALA:H	1.29	0.94
1:B:9:ILE:HG21	1:B:31:TYR:CD2	2.02	0.93
1:A:74:MET:HE2	1:A:96:ILE:CD1	1.98	0.93
1:A:53:TYR:HE1	1:A:78:ASN:CG	1.75	0.93
1:B:218:ASN:ND2	1:B:218:ASN:C	2.26	0.93
1:A:25:LYS:NZ	1:A:25:LYS:CB	2.32	0.92
1:A:3:LYS:CG	1:A:47:ALA:CB	2.48	0.92
1:A:3:LYS:CD	1:A:47:ALA:HB2	1.99	0.92
1:B:75:SER:OG	1:B:97:THR:OG1	1.87	0.92
1:A:53:TYR:HE1	1:A:78:ASN:CB	1.77	0.91
1:A:210:VAL:CG1	1:A:212:ALA:H	1.83	0.91
1:B:81:VAL:HG12	1:B:84:ILE:CD1	2.00	0.90
1:A:278:PHE:CE2	1:A:284:ALA:HB2	2.07	0.90
1:B:133:ASP:OD1	1:B:135:ARG:HG2	1.70	0.90
1:A:306:VAL:CA	1:A:309:MET:HG3	2.02	0.89
1:B:21:LYS:HE2	1:B:21:LYS:C	1.96	0.89
1:A:113:ILE:CD1	1:B:116:ALA:HB1	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:MET:HB3	1:B:332:LEU:HG	1.53	0.89
1:B:90:LYS:HB2	1:B:332:LEU:CD1	2.03	0.89
1:A:149:VAL:CG2	1:A:165:MET:HE3	2.03	0.89
2:B:401:NAI:H5N	3:B:402:OXM:HN2	1.16	0.88
1:B:82:ASP:HA	1:B:336:LYS:HG2	1.55	0.88
1:A:7:TYR:CD2	1:A:36:LEU:HD12	2.09	0.88
1:B:87:ASP:O	1:B:91:GLU:N	2.06	0.88
1:B:207:VAL:CG1	1:B:216:MET:HE1	2.03	0.88
1:A:113:ILE:HD11	1:B:116:ALA:HB1	1.56	0.87
1:B:82:ASP:HA	1:B:336:LYS:CG	2.04	0.87
1:B:207:VAL:HG11	1:B:216:MET:HE1	1.55	0.87
1:A:25:LYS:HZ2	1:A:25:LYS:HB3	1.37	0.87
1:B:54:GLN:HE21	1:B:56:LEU:C	1.83	0.87
1:A:306:VAL:HA	1:A:309:MET:CG	2.03	0.86
1:B:10:ARG:NH2	1:B:306:VAL:HG13	1.90	0.86
1:B:1:MET:HG3	1:B:2:THR:H	1.34	0.86
1:A:7:TYR:CE2	1:A:36:LEU:HD12	2.11	0.85
1:B:86:MET:HE3	1:B:332:LEU:HG	1.56	0.85
1:A:9:ILE:CD1	1:A:77:ARG:NH1	2.40	0.85
1:B:262:TYR:HB3	1:B:265:GLU:HB3	1.59	0.84
1:B:57:ASP:OD1	1:B:57:ASP:N	2.10	0.84
1:A:21:LYS:HA	1:A:21:LYS:CE	2.00	0.84
1:A:85:ASP:O	1:A:89:ALA:HB2	1.77	0.84
1:B:35:LEU:HD23	1:B:35:LEU:H	1.39	0.84
1:B:63:LEU:HD12	1:B:63:LEU:H	1.41	0.84
1:B:213:ASN:HD21	2:B:401:NAI:H61A	1.25	0.84
1:B:257:PHE:CZ	1:B:259:MET:HE3	2.13	0.84
1:A:285:ASP:OD2	1:A:289:ARG:NH1	2.12	0.83
1:B:332:LEU:C	1:B:332:LEU:CD2	2.51	0.83
2:A:401:NAI:H42N	3:A:402:OXM:C1	2.09	0.83
1:B:218:ASN:HD21	1:B:220:LYS:H	1.22	0.83
1:A:6:ALA:HB3	1:A:31:TYR:HB3	1.59	0.83
1:B:48:ASP:O	1:B:73:LYS:HD2	1.78	0.83
1:B:114:GLN:O	1:B:118:VAL:HG23	1.78	0.83
1:B:297:HIS:NE2	3:B:402:OXM:O1	2.12	0.82
1:B:219:ASP:CG	1:B:247:ARG:HH12	1.87	0.82
1:B:86:MET:CE	1:B:332:LEU:CA	2.56	0.82
1:A:295:THR:HG22	1:A:296:PRO:HD2	1.60	0.82
1:B:287:ILE:HA	1:B:294:VAL:HG21	1.59	0.82
1:A:25:LYS:CB	1:A:25:LYS:HZ2	1.91	0.81
1:B:64:GLN:HA	1:B:67:ALA:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:VAL:HG12	1:B:212:ALA:H	1.45	0.81
1:B:63:LEU:H	1:B:63:LEU:CD1	1.93	0.81
1:A:297:HIS:NE2	3:A:402:OXM:O1	2.14	0.81
1:B:21:LYS:HE2	1:B:21:LYS:HA	1.61	0.81
1:A:210:VAL:HG12	1:A:213:ASN:H	1.45	0.81
1:A:74:MET:O	1:A:96:ILE:HA	1.80	0.81
1:A:190:VAL:HG11	1:A:195:ASP:CB	2.11	0.81
1:B:162:MET:CE	1:B:172:VAL:CG1	2.60	0.80
1:A:53:TYR:CE1	1:A:78:ASN:CG	2.55	0.80
1:A:319:LYS:NZ	1:A:324:GLU:OE1	2.14	0.80
1:A:149:VAL:HG21	1:A:165:MET:CE	2.10	0.80
1:A:64:GLN:HA	1:A:67:ALA:HB3	1.63	0.80
1:A:2:THR:O	1:A:28:ASP:HB3	1.80	0.80
1:A:3:LYS:CG	1:A:47:ALA:HB2	2.11	0.80
1:B:151:VAL:CG2	1:B:162:MET:HE3	2.12	0.80
1:B:155:GLY:O	1:B:156:HIS:C	2.24	0.80
1:B:63:LEU:N	1:B:63:LEU:CD1	2.45	0.79
1:A:7:TYR:CG	1:A:36:LEU:HD12	2.18	0.79
1:A:5:PHE:HE1	1:A:30:ASP:HB3	1.47	0.79
1:A:38:PRO:HG3	1:A:62:THR:OG1	1.82	0.79
1:B:213:ASN:ND2	2:B:401:NAI:N6A	2.31	0.79
1:B:110:HIS:O	1:B:114:GLN:HG2	1.82	0.79
1:A:190:VAL:CG1	1:A:195:ASP:HB2	2.12	0.79
1:B:219:ASP:OD2	1:B:247:ARG:NH1	2.16	0.78
1:B:287:ILE:HA	1:B:294:VAL:CG2	2.13	0.78
1:B:319:LYS:HZ2	1:B:324:GLU:HB3	1.48	0.78
1:B:218:ASN:ND2	1:B:220:LYS:N	2.32	0.78
1:A:102:TYR:HB2	1:A:305:ALA:HB1	1.66	0.78
1:A:229:VAL:HG22	1:A:230:VAL:N	1.99	0.77
1:A:84:ILE:HD11	1:A:86:MET:SD	2.24	0.77
1:A:178:PHE:O	1:A:178:PHE:CD1	2.37	0.77
1:B:319:LYS:NZ	1:B:324:GLU:HB3	2.00	0.77
1:B:35:LEU:N	1:B:35:LEU:CD2	2.48	0.77
1:A:267:GLY:O	1:A:271:LYS:NZ	2.12	0.77
1:B:277:GLU:O	1:B:279:PRO:HD3	1.85	0.77
1:A:14:GLU:CB	1:A:15:PRO:HD3	2.15	0.76
1:B:29:VAL:O	1:B:30:ASP:OD1	2.02	0.76
1:A:186:LYS:HB2	1:A:186:LYS:NZ	1.97	0.76
1:A:318:LEU:O	1:A:318:LEU:HD23	1.85	0.76
1:B:332:LEU:CD2	1:B:332:LEU:O	2.33	0.76
1:A:10:ARG:HB2	1:A:13:GLU:HG3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ARG:O	1:B:307:ARG:HG2	1.85	0.76
1:A:14:GLU:HB2	1:A:15:PRO:HD3	1.68	0.76
1:A:6:ALA:HB1	1:A:9:ILE:HD13	1.67	0.76
1:A:9:ILE:HD12	1:A:77:ARG:HH12	1.49	0.76
1:B:151:VAL:HG21	1:B:162:MET:HE3	1.68	0.75
1:B:177:ILE:CG2	1:B:178:PHE:N	2.48	0.75
1:A:156:HIS:CD2	1:A:157:ILE:H	2.04	0.75
1:A:6:ALA:HB1	1:A:9:ILE:CD1	2.17	0.75
1:B:54:GLN:NE2	1:B:56:LEU:CB	2.50	0.75
1:B:156:HIS:CD2	2:B:401:NAI:O1N	2.40	0.75
1:A:210:VAL:CG2	1:A:211:PRO:HD2	2.16	0.75
1:A:273:TRP:CZ3	1:A:279:PRO:HG3	2.21	0.75
1:B:17:LEU:C	1:B:18:ASN:HD22	1.95	0.75
1:B:273:TRP:CZ3	1:B:279:PRO:HG3	2.22	0.75
1:A:59:THR:O	1:A:63:LEU:HD13	1.85	0.75
1:A:207:VAL:CG1	1:A:216:MET:HE1	2.16	0.75
1:A:219:ASP:OD1	1:A:247:ARG:NH1	2.19	0.74
1:B:210:VAL:HG13	1:B:211:PRO:HD2	1.68	0.74
1:B:25:LYS:HA	1:B:25:LYS:HE2	1.69	0.74
1:A:4:VAL:CG1	1:A:317:ASN:HD22	2.01	0.74
1:B:99:VAL:HG12	1:B:99:VAL:O	1.86	0.74
1:A:310:VAL:O	1:A:313:ALA:CB	2.35	0.74
1:A:17:LEU:HD12	1:A:314:PHE:HZ	1.52	0.74
1:B:54:GLN:HE21	1:B:56:LEU:CA	2.01	0.74
1:B:154:THR:HG21	1:B:183:LEU:CD2	2.17	0.74
2:B:401:NAI:H42N	3:B:402:OXM:C1	2.18	0.73
1:A:139:THR:HG22	1:A:139:THR:O	1.87	0.73
1:A:43:LEU:C	1:A:45:LYS:H	1.96	0.73
1:B:40:THR:O	1:B:42:LYS:N	2.21	0.73
1:B:88:LYS:O	1:B:89:ALA:C	2.32	0.73
1:A:245:VAL:CG1	1:A:254:ILE:HD12	2.18	0.73
1:A:2:THR:O	1:A:28:ASP:CB	2.36	0.72
1:A:154:THR:O	1:A:154:THR:HG22	1.90	0.72
1:A:317:ASN:O	1:A:320:LEU:N	2.22	0.72
1:B:10:ARG:HH22	1:B:306:VAL:HG13	1.52	0.72
1:B:98:ASN:HD21	1:B:328:SER:HB3	1.54	0.72
1:B:319:LYS:HD2	1:B:326:PRO:HA	1.72	0.72
1:A:48:ASP:HB3	1:A:321:ILE:HG12	1.71	0.72
1:B:222:ILE:HA	1:B:225:MET:SD	2.29	0.72
1:B:335:ASN:ND2	1:B:337:PHE:OXT	2.22	0.72
1:B:21:LYS:HG2	1:B:29:VAL:HG21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ASP:O	1:B:90:LYS:N	2.22	0.72
1:A:207:VAL:HG11	1:A:216:MET:HE1	1.70	0.72
1:A:3:LYS:O	1:A:48:ASP:N	2.23	0.71
1:B:103:SER:OG	1:B:103:SER:O	2.06	0.71
1:B:21:LYS:HE2	1:B:21:LYS:O	1.89	0.71
1:A:47:ALA:O	1:A:71:VAL:HG22	1.91	0.71
1:A:88:LYS:HA	1:A:91:GLU:HB2	1.71	0.71
1:A:177:ILE:HG22	1:A:178:PHE:N	2.06	0.71
1:B:125:MET:HE3	1:B:128:LYS:CE	2.20	0.71
1:B:217:ILE:HA	1:B:221:SER:OG	1.90	0.71
2:B:401:NAI:C4N	3:B:402:OXM:C1	2.69	0.71
1:A:6:ALA:HA	1:A:51:VAL:O	1.91	0.71
1:B:151:VAL:HG21	1:B:162:MET:HG2	1.72	0.71
1:B:213:ASN:HB3	1:B:216:MET:HE2	1.71	0.71
1:A:20:TRP:CE3	1:A:20:TRP:C	2.69	0.71
1:A:259:MET:HG2	1:A:294:VAL:HG22	1.73	0.71
1:A:49:GLY:HA2	1:A:73:LYS:O	1.90	0.70
1:A:210:VAL:CG1	1:A:212:ALA:N	2.54	0.70
1:B:218:ASN:HD21	1:B:220:LYS:N	1.88	0.70
1:B:98:ASN:C	1:B:98:ASN:HD22	1.98	0.70
1:A:136:TRP:O	1:B:301:TYR:CE2	2.44	0.70
1:A:144:VAL:O	1:A:146:ASP:N	2.24	0.70
1:A:273:TRP:CE3	1:A:279:PRO:HG3	2.25	0.70
1:A:7:TYR:CZ	1:A:36:LEU:HD12	2.26	0.70
1:A:99:VAL:O	1:A:99:VAL:HG12	1.90	0.70
1:A:176:ASP:OD2	2:A:401:NAI:H4B	1.90	0.70
1:A:5:PHE:CE1	1:A:30:ASP:HB3	2.26	0.70
1:B:23:ALA:O	1:B:25:LYS:HG2	1.91	0.70
1:A:236:ARG:O	1:A:239:LEU:HG	1.92	0.69
1:B:278:PHE:CD1	1:B:279:PRO:HD2	2.25	0.69
1:B:177:ILE:HG22	1:B:178:PHE:H	1.57	0.69
1:B:20:TRP:CE2	1:B:24:HIS:CD2	2.81	0.69
1:B:48:ASP:HB3	1:B:321:ILE:CD1	2.23	0.69
1:B:81:VAL:CB	1:B:84:ILE:HD11	2.22	0.69
1:B:236:ARG:HG2	2:B:401:NAI:O2D	1.92	0.69
1:A:270:ASN:HA	1:B:134:LEU:O	1.93	0.69
1:B:36:LEU:HD11	1:B:41:ALA:HB2	1.73	0.69
1:B:154:THR:O	1:B:154:THR:CG2	2.40	0.69
1:B:32:THR:HG23	1:B:33:ASP:N	2.07	0.69
1:A:113:ILE:O	1:A:117:ARG:HG3	1.92	0.69
1:B:14:GLU:HB3	1:B:15:PRO:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HD13	1:B:54:GLN:HG3	1.74	0.69
1:B:142:ARG:HH11	1:B:147:GLN:HE21	1.40	0.69
1:B:257:PHE:HZ	1:B:259:MET:HE3	1.54	0.69
1:B:285:ASP:OD2	1:B:289:ARG:NH1	2.25	0.69
1:B:308:ASN:O	1:B:312:LYS:HB2	1.94	0.68
1:A:74:MET:CE	1:A:96:ILE:CD1	2.69	0.68
1:A:74:MET:CE	1:A:96:ILE:HD11	2.22	0.68
1:B:14:GLU:HB3	1:B:15:PRO:CD	2.24	0.68
1:A:2:THR:CB	1:A:27:ILE:HG23	2.22	0.68
1:A:142:ARG:HH11	1:A:147:GLN:HE21	1.42	0.68
1:B:125:MET:HE3	1:B:128:LYS:HE3	1.74	0.68
1:B:157:ILE:CD1	2:B:401:NAI:H51N	2.21	0.68
1:B:74:MET:O	1:B:96:ILE:CG2	2.38	0.67
1:B:262:TYR:O	1:B:265:GLU:HB3	1.93	0.67
1:B:87:ASP:N	1:B:87:ASP:OD1	2.26	0.67
1:B:9:ILE:HG21	1:B:31:TYR:CE2	2.28	0.67
1:B:86:MET:HE3	1:B:332:LEU:CG	2.24	0.67
1:A:218:ASN:ND2	1:A:220:LYS:H	1.92	0.67
1:A:9:ILE:HG21	1:A:31:TYR:CE2	2.30	0.67
1:A:162:MET:HG2	1:A:172:VAL:HG11	1.75	0.67
1:B:27:ILE:CD1	1:B:318:LEU:HD11	2.24	0.67
1:B:219:ASP:CG	1:B:247:ARG:NH1	2.53	0.67
1:B:214:VAL:HG13	1:B:238:ARG:HB3	1.77	0.67
1:A:136:TRP:O	1:B:301:TYR:HE2	1.76	0.67
1:B:222:ILE:O	1:B:225:MET:CB	2.37	0.67
1:B:192:SER:O	1:B:195:ASP:HB2	1.95	0.66
1:B:89:ALA:O	1:B:93:GLY:N	2.28	0.66
1:A:8:ALA:HB2	1:A:35:LEU:HD22	1.76	0.66
1:A:229:VAL:CG2	1:A:230:VAL:N	2.57	0.66
1:B:2:THR:CB	1:B:27:ILE:HG23	2.22	0.66
1:A:305:ALA:O	1:A:308:ASN:N	2.29	0.66
1:B:54:GLN:HE21	1:B:56:LEU:CB	2.08	0.66
1:A:123:LYS:HE2	1:A:290:PRO:HA	1.77	0.66
1:A:182:GLU:C	1:A:182:GLU:CD	2.64	0.66
1:B:102:TYR:HD2	1:B:309:MET:HG3	1.61	0.66
1:A:250:ASP:OD1	1:A:289:ARG:NH2	2.28	0.66
1:A:35:LEU:HD13	1:A:54:GLN:CG	2.25	0.66
1:A:74:MET:HE2	1:A:96:ILE:HD11	1.78	0.66
1:A:101:VAL:HG12	1:A:101:VAL:O	1.95	0.66
1:B:282:ARG:O	1:B:283:LEU:C	2.38	0.66
1:A:310:VAL:HG12	1:A:311:VAL:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:THR:HA	1:A:65:ALA:HB3	1.78	0.65
1:B:142:ARG:NH1	1:B:147:GLN:HE21	1.94	0.65
1:B:241:ASP:O	1:B:244:ALA:N	2.28	0.65
1:B:54:GLN:HG2	1:B:56:LEU:H	1.60	0.65
1:B:64:GLN:HA	1:B:67:ALA:CB	2.25	0.65
1:A:7:TYR:O	1:A:52:VAL:HA	1.97	0.65
1:A:319:LYS:NZ	1:A:324:GLU:CB	2.59	0.65
1:B:317:ASN:O	1:B:320:LEU:HB2	1.96	0.65
1:A:48:ASP:O	1:A:71:VAL:HG13	1.97	0.65
1:B:7:TYR:OH	1:B:43:LEU:HB3	1.97	0.65
1:B:63:LEU:O	1:B:66:LEU:HB3	1.97	0.65
1:B:316:ASN:HD21	1:B:327:ASP:C	2.05	0.65
1:B:9:ILE:CG2	1:B:9:ILE:O	2.45	0.65
1:B:193:LEU:HG	1:B:197:TYR:CE1	2.32	0.65
1:A:7:TYR:CG	1:A:36:LEU:CD1	2.80	0.65
1:A:162:MET:HB2	1:A:163:ARG:NH1	2.12	0.65
1:B:85:ASP:OD2	1:B:88:LYS:CB	2.39	0.65
1:B:98:ASN:C	1:B:98:ASN:ND2	2.54	0.65
1:A:210:VAL:HG13	1:A:211:PRO:CD	2.26	0.64
1:A:3:LYS:HB3	1:A:47:ALA:CA	2.18	0.64
1:A:108:ALA:HB3	1:A:160:VAL:HG11	1.78	0.64
1:A:209:ASP:C	1:A:209:ASP:OD1	2.39	0.64
1:B:14:GLU:N	1:B:15:PRO:HD2	2.13	0.64
1:B:39:GLU:OE1	1:B:39:GLU:O	2.15	0.64
1:B:123:LYS:HD3	1:B:290:PRO:O	1.96	0.64
1:A:154:THR:O	1:A:154:THR:CG2	2.45	0.64
1:A:3:LYS:CG	1:A:47:ALA:HB1	2.14	0.64
1:A:102:TYR:HA	1:A:308:ASN:HD22	1.62	0.64
1:A:260:ASP:OD1	1:A:297:HIS:HA	1.96	0.64
1:A:52:VAL:O	1:A:76:LEU:HD13	1.98	0.64
2:A:401:NAI:H42N	3:A:402:OXM:N1	2.11	0.64
1:B:142:ARG:NH2	1:B:228:GLY:O	2.30	0.64
1:A:190:VAL:CG1	1:A:195:ASP:CB	2.74	0.64
1:A:205:LEU:N	1:A:205:LEU:HD13	2.12	0.64
1:B:98:ASN:ND2	1:B:328:SER:HB3	2.13	0.64
1:B:332:LEU:O	1:B:332:LEU:HD22	1.97	0.64
1:B:82:ASP:HA	1:B:336:LYS:HG3	1.79	0.64
1:A:229:VAL:CG2	1:A:230:VAL:H	2.11	0.63
1:B:86:MET:HG2	1:B:336:LYS:HD3	1.81	0.63
1:B:23:ALA:O	1:B:25:LYS:N	2.31	0.63
1:A:90:LYS:HD2	1:A:90:LYS:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:THR:HG22	1:B:3:LYS:N	2.12	0.63
1:B:102:TYR:CD2	1:B:309:MET:HG3	2.33	0.63
1:B:317:ASN:O	1:B:320:LEU:N	2.30	0.63
1:A:9:ILE:CG2	1:A:31:TYR:CD2	2.80	0.63
1:A:267:GLY:C	1:A:271:LYS:HZ2	2.04	0.63
1:B:38:PRO:HA	1:B:65:ALA:CB	2.29	0.63
1:B:86:MET:HE1	1:B:332:LEU:HA	1.76	0.63
1:A:2:THR:HB	1:A:27:ILE:CG2	2.26	0.63
1:A:3:LYS:HG2	1:A:47:ALA:HB2	1.66	0.63
1:A:3:LYS:CB	1:A:47:ALA:HA	2.18	0.63
1:B:63:LEU:O	1:B:66:LEU:N	2.32	0.63
1:A:281:LYS:O	1:A:285:ASP:N	2.31	0.63
1:A:35:LEU:HD13	1:A:54:GLN:HG3	1.81	0.62
1:A:113:ILE:HD13	1:B:116:ALA:CB	2.29	0.62
1:B:102:TYR:CD2	1:B:309:MET:CG	2.81	0.62
1:A:2:THR:HG21	1:A:321:ILE:HG21	1.79	0.62
1:A:73:LYS:HD2	1:A:321:ILE:HA	1.81	0.62
1:A:108:ALA:CB	1:A:160:VAL:CG1	2.78	0.62
1:A:196:LEU:C	1:A:196:LEU:HD23	2.24	0.62
1:A:317:ASN:O	1:A:318:LEU:C	2.40	0.62
1:B:21:LYS:HA	1:B:21:LYS:CE	2.29	0.62
1:B:39:GLU:OE1	1:B:39:GLU:C	2.41	0.62
1:A:278:PHE:CD1	1:A:279:PRO:HD2	2.34	0.62
1:B:184:GLU:HA	1:B:189:TYR:HD1	1.63	0.62
1:A:278:PHE:HE2	1:A:284:ALA:HB2	1.65	0.62
1:B:54:GLN:NE2	1:B:56:LEU:C	2.50	0.62
1:B:319:LYS:CB	1:B:326:PRO:HB3	2.30	0.62
1:B:319:LYS:CD	1:B:326:PRO:HA	2.29	0.62
1:A:98:ASN:ND2	1:A:100:PRO:HD3	2.15	0.62
1:A:300:PHE:C	1:A:300:PHE:CD1	2.78	0.62
1:B:17:LEU:HB3	1:B:18:ASN:ND2	2.14	0.62
1:B:87:ASP:O	1:B:88:LYS:C	2.41	0.62
1:B:88:LYS:O	1:B:92:LEU:N	2.17	0.62
1:A:25:LYS:NZ	1:A:25:LYS:C	2.58	0.61
1:A:4:VAL:CG1	1:A:317:ASN:ND2	2.63	0.61
1:B:13:GLU:OE1	1:B:77:ARG:NH2	2.33	0.61
1:A:50:VAL:N	1:A:73:LYS:O	2.32	0.61
1:A:60:ALA:HB2	1:A:85:ASP:OD2	1.99	0.61
1:A:283:LEU:O	1:A:287:ILE:HG13	2.01	0.61
1:A:330:VAL:HG12	1:A:330:VAL:O	1.98	0.61
1:B:297:HIS:HE2	3:B:402:OXM:C1	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:VAL:C	1:A:313:ALA:N	2.56	0.61
1:B:159:GLN:O	1:B:162:MET:HB2	2.01	0.61
1:B:25:LYS:HA	1:B:25:LYS:CE	2.30	0.61
1:B:29:VAL:O	1:B:30:ASP:CG	2.43	0.61
1:A:31:TYR:HD1	1:A:31:TYR:H	1.47	0.61
1:A:222:ILE:HA	1:A:225:MET:SD	2.41	0.61
1:B:18:ASN:O	1:B:22:GLU:HB2	2.00	0.61
1:B:218:ASN:O	1:B:222:ILE:HG13	2.01	0.61
1:A:2:THR:CG2	1:A:321:ILE:HG21	2.31	0.61
1:A:7:TYR:CD1	1:A:36:LEU:HD12	2.34	0.61
1:A:21:LYS:HG3	1:A:29:VAL:HB	1.82	0.61
1:A:186:LYS:HE2	1:A:188:TYR:CE2	2.36	0.61
1:A:319:LYS:HZ1	1:A:324:GLU:CB	2.14	0.61
1:A:331:ALA:O	1:A:333:ASN:N	2.34	0.61
1:B:86:MET:O	1:B:332:LEU:HD12	2.01	0.61
1:B:327:ASP:O	1:B:328:SER:CB	2.47	0.61
1:A:20:TRP:CE3	1:A:20:TRP:O	2.53	0.60
1:A:113:ILE:CD1	1:B:116:ALA:CB	2.75	0.60
1:B:316:ASN:OD1	1:B:327:ASP:N	2.29	0.60
1:A:162:MET:CB	1:A:163:ARG:NH1	2.64	0.60
1:A:49:GLY:CA	1:A:73:LYS:O	2.49	0.60
1:B:54:GLN:HG2	1:B:55:GLN:N	2.14	0.60
1:A:182:GLU:OE1	1:A:183:LEU:CD1	2.50	0.60
1:A:242:THR:O	1:A:246:ILE:HG13	2.02	0.60
1:B:25:LYS:HE2	1:B:25:LYS:CA	2.32	0.60
1:A:74:MET:HE2	1:A:96:ILE:HD13	1.80	0.60
1:B:12:ASP:O	1:B:15:PRO:HG2	2.02	0.60
1:A:113:ILE:HD13	1:B:116:ALA:HB1	1.83	0.60
1:A:260:ASP:HA	1:A:295:THR:O	2.01	0.60
1:B:142:ARG:HD2	1:B:147:GLN:HE22	1.67	0.60
1:A:210:VAL:O	1:A:214:VAL:HG23	2.02	0.60
1:A:19:GLU:CA	1:A:22:GLU:OE1	2.39	0.60
1:A:197:TYR:O	1:A:225:MET:HA	2.01	0.60
1:B:315:ASN:O	1:B:318:LEU:N	2.35	0.60
1:A:8:ALA:C	1:A:77:ARG:HH22	2.10	0.59
1:A:192:SER:O	1:A:195:ASP:HB2	2.02	0.59
1:B:21:LYS:HG2	1:B:29:VAL:CG2	2.32	0.59
1:A:96:ILE:HG22	1:A:330:VAL:HG23	1.80	0.59
1:A:261:THR:HG23	1:A:265:GLU:OE1	2.02	0.59
1:A:318:LEU:O	1:A:322:ASN:HB2	2.02	0.59
1:A:7:TYR:CE1	1:A:36:LEU:HD12	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LYS:HZ1	1:A:324:GLU:HB3	1.65	0.59
1:B:97:THR:HG21	1:B:316:ASN:HB3	1.84	0.59
1:B:138:PRO:O	1:B:140:ILE:HG22	2.02	0.59
1:B:240:VAL:HG12	1:B:241:ASP:N	2.17	0.59
1:A:5:PHE:CZ	1:A:31:TYR:O	2.55	0.59
1:B:90:LYS:HZ2	1:B:93:GLY:HA2	1.67	0.59
1:A:5:PHE:CD1	1:A:30:ASP:O	2.55	0.59
1:A:58:TYR:CD2	1:A:84:ILE:CG2	2.86	0.59
1:A:209:ASP:OD1	1:A:209:ASP:O	2.21	0.59
1:A:210:VAL:HG12	1:A:212:ALA:N	2.17	0.59
1:B:86:MET:HE3	1:B:332:LEU:CB	2.33	0.59
1:B:11:LYS:O	1:B:15:PRO:HD2	2.03	0.59
1:B:18:ASN:O	1:B:22:GLU:CB	2.51	0.59
1:A:260:ASP:CG	1:A:298:THR:H	2.10	0.59
1:B:20:TRP:HE3	1:B:21:LYS:N	2.01	0.59
1:A:102:TYR:HB2	1:A:305:ALA:CB	2.31	0.58
1:A:142:ARG:NH2	1:A:228:GLY:O	2.35	0.58
1:A:152:VAL:O	1:A:206:HIS:N	2.34	0.58
1:A:331:ALA:O	1:A:332:LEU:C	2.46	0.58
1:B:207:VAL:HG22	1:B:208:PRO:CD	2.32	0.58
1:B:5:PHE:O	1:B:50:VAL:HA	2.03	0.58
1:B:36:LEU:HD13	1:B:41:ALA:HA	1.84	0.58
1:A:323:GLY:O	1:A:324:GLU:HG3	2.02	0.58
1:B:297:HIS:CD2	3:B:402:OXM:O1	2.55	0.58
1:A:311:VAL:C	1:A:313:ALA:H	2.10	0.58
1:A:280:ASP:C	1:A:280:ASP:OD1	2.47	0.58
1:B:125:MET:O	1:B:128:LYS:N	2.34	0.58
1:B:151:VAL:HG23	1:B:162:MET:HE3	1.82	0.58
1:A:154:THR:HG21	1:A:189:TYR:OH	2.04	0.58
1:B:90:LYS:NZ	1:B:93:GLY:HA2	2.18	0.58
1:A:31:TYR:CD1	1:A:31:TYR:N	2.72	0.58
1:A:209:ASP:HA	1:A:239:LEU:HD21	1.86	0.58
1:A:297:HIS:CD2	3:A:402:OXM:O1	2.57	0.58
1:B:135:ARG:HG3	1:B:135:ARG:HH11	1.67	0.58
1:B:36:LEU:HD12	1:B:37:THR:H	1.63	0.57
1:B:210:VAL:C	1:B:212:ALA:N	2.61	0.57
1:B:285:ASP:O	1:B:289:ARG:HG2	2.03	0.57
1:B:86:MET:HE2	1:B:332:LEU:CA	2.18	0.57
1:A:210:VAL:HG13	1:A:211:PRO:N	2.18	0.57
1:A:214:VAL:HG12	1:A:214:VAL:O	2.03	0.57
1:B:42:LYS:NZ	1:B:42:LYS:HB3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:O	1:A:67:ALA:N	2.27	0.57
1:A:125:MET:HE2	1:B:296:PRO:CD	2.35	0.57
1:B:86:MET:SD	1:B:336:LYS:HE2	2.45	0.57
1:B:278:PHE:CE2	1:B:284:ALA:HB2	2.39	0.57
1:A:201:ASP:OD1	1:A:226:LYS:NZ	2.32	0.57
1:B:173:ILE:HD11	1:B:199:GLN:HG3	1.87	0.57
1:A:96:ILE:O	1:A:330:VAL:HB	2.04	0.57
1:A:125:MET:HE2	1:B:296:PRO:HD3	1.87	0.57
1:A:281:LYS:HD2	1:A:281:LYS:C	2.30	0.57
1:B:77:ARG:HG3	1:B:313:ALA:CB	2.35	0.57
1:B:181:PRO:HA	1:B:184:GLU:OE2	2.05	0.57
1:A:20:TRP:CE2	1:A:314:PHE:HB3	2.39	0.57
1:A:186:LYS:HB2	1:A:186:LYS:HZ3	1.69	0.57
1:A:301:TYR:OH	1:B:138:PRO:HA	2.04	0.57
1:A:213:ASN:ND2	2:A:401:NAI:N6A	2.52	0.56
1:A:315:ASN:O	1:A:318:LEU:N	2.38	0.56
1:A:135:ARG:HG3	1:A:135:ARG:HH11	1.70	0.56
1:B:28:ASP:OD1	1:B:29:VAL:N	2.39	0.56
1:B:48:ASP:HB3	1:B:321:ILE:HG12	1.86	0.56
1:A:58:TYR:CD2	1:A:84:ILE:HG23	2.40	0.56
1:A:143:GLU:OE2	1:B:302:THR:HG21	2.06	0.56
1:A:235:SER:HA	2:A:401:NAI:H1D	1.87	0.56
1:A:270:ASN:HA	1:B:135:ARG:HA	1.87	0.56
1:B:42:LYS:HB3	1:B:42:LYS:HZ2	1.69	0.56
1:B:319:LYS:HB3	1:B:326:PRO:HB3	1.88	0.56
1:A:7:TYR:CD1	1:A:36:LEU:CD1	2.88	0.56
1:A:245:VAL:HG13	1:A:254:ILE:HD13	1.82	0.56
1:A:263:GLU:HG3	1:A:264:ASP:OD1	2.05	0.56
1:B:27:ILE:HD12	1:B:318:LEU:HD11	1.87	0.56
1:B:235:SER:HA	2:B:401:NAI:H1D	1.88	0.56
1:A:81:VAL:O	1:A:84:ILE:HG13	2.05	0.56
1:A:108:ALA:HB1	1:A:160:VAL:HG12	1.88	0.56
1:B:10:ARG:NH2	1:B:306:VAL:CG1	2.65	0.56
1:B:38:PRO:HA	1:B:65:ALA:HB1	1.88	0.56
1:A:64:GLN:HA	1:A:67:ALA:CB	2.36	0.56
2:B:401:NAI:C4N	3:B:402:OXM:N1	2.66	0.56
1:B:142:ARG:HH11	1:B:147:GLN:NE2	2.03	0.56
1:A:205:LEU:N	1:A:205:LEU:CD1	2.68	0.56
1:B:35:LEU:CD1	1:B:54:GLN:HG3	2.36	0.56
1:B:173:ILE:CD1	1:B:199:GLN:HG3	2.36	0.56
1:B:297:HIS:NE2	2:B:401:NAI:H42N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:MET:CG	1:B:336:LYS:HD3	2.36	0.55
1:A:21:LYS:CA	1:A:21:LYS:CE	2.70	0.55
1:A:21:LYS:CG	1:A:29:VAL:HB	2.36	0.55
1:A:182:GLU:OE1	1:A:183:LEU:HD13	2.06	0.55
1:B:157:ILE:HD12	2:B:401:NAI:C5D	2.26	0.55
1:B:259:MET:HG3	1:B:261:THR:O	2.05	0.55
1:A:14:GLU:CB	1:A:15:PRO:CD	2.83	0.55
1:A:210:VAL:CB	1:A:211:PRO:HD2	2.37	0.55
1:A:281:LYS:O	1:A:284:ALA:N	2.40	0.55
1:A:329:PRO:O	1:A:332:LEU:CD2	2.55	0.55
1:B:321:ILE:HG22	1:B:322:ASN:N	2.22	0.55
1:A:17:LEU:HD12	1:A:314:PHE:CZ	2.36	0.55
1:A:319:LYS:HZ2	1:A:324:GLU:HB2	1.71	0.55
1:B:190:VAL:HG13	1:B:195:ASP:HB2	1.88	0.55
1:B:210:VAL:O	1:B:214:VAL:HG23	2.07	0.55
1:A:82:ASP:OD1	1:A:82:ASP:C	2.49	0.55
1:A:143:GLU:O	1:A:147:GLN:OE1	2.25	0.55
1:B:58:TYR:CD2	1:B:84:ILE:HG23	2.42	0.55
1:A:38:PRO:O	1:A:65:ALA:HB1	2.07	0.55
1:B:66:LEU:CD2	1:B:94:PHE:HZ	2.08	0.55
1:B:210:VAL:CG1	1:B:211:PRO:HD2	2.37	0.55
1:B:332:LEU:HD23	1:B:332:LEU:O	1.98	0.55
1:B:334:LYS:HD2	1:B:334:LYS:N	2.21	0.55
1:A:73:LYS:CD	1:A:321:ILE:HA	2.37	0.55
1:A:219:ASP:CG	1:A:247:ARG:NH1	2.65	0.55
1:B:90:LYS:O	1:B:93:GLY:N	2.40	0.55
1:B:222:ILE:HD13	1:B:254:ILE:HD11	1.89	0.55
1:A:86:MET:O	1:A:89:ALA:HB3	2.07	0.55
1:B:18:ASN:O	1:B:22:GLU:N	2.35	0.55
1:A:48:ASP:O	1:A:73:LYS:HB2	2.07	0.55
1:A:145:ARG:HB2	1:A:168:PHE:O	2.07	0.55
1:A:4:VAL:HG13	1:A:317:ASN:HD22	1.72	0.54
1:A:283:LEU:O	1:A:283:LEU:HD12	2.06	0.54
1:A:319:LYS:NZ	1:A:324:GLU:CD	2.64	0.54
1:B:194:ASP:O	1:B:198:LYS:HG2	2.07	0.54
1:A:20:TRP:CZ3	1:A:29:VAL:HG21	2.42	0.54
1:A:305:ALA:O	1:A:306:VAL:C	2.49	0.54
1:A:319:LYS:NZ	1:A:324:GLU:HB3	2.22	0.54
1:A:5:PHE:HD2	1:A:7:TYR:CE1	2.26	0.54
1:B:90:LYS:O	1:B:91:GLU:C	2.45	0.54
1:B:173:ILE:HD11	1:B:199:GLN:NE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:TYR:O	1:B:225:MET:HA	2.07	0.54
1:B:214:VAL:O	1:B:215:HIS:HB2	2.07	0.54
1:A:96:ILE:CG2	1:A:97:THR:N	2.71	0.54
1:B:90:LYS:O	1:B:90:LYS:HD2	2.08	0.54
1:B:286:LEU:O	1:B:287:ILE:C	2.51	0.54
1:A:277:GLU:OE1	1:A:277:GLU:CA	2.37	0.54
1:B:64:GLN:O	1:B:68:ASP:OD1	2.26	0.54
1:A:11:LYS:NZ	1:A:14:GLU:CD	2.65	0.54
1:A:24:HIS:CE1	1:A:318:LEU:HD12	2.43	0.54
1:A:37:THR:OG1	1:A:40:THR:N	2.39	0.54
1:A:59:THR:HB	1:A:61:ASP:OD2	2.07	0.54
1:B:210:VAL:O	1:B:212:ALA:N	2.41	0.54
1:A:54:GLN:HB2	1:A:58:TYR:OH	2.08	0.54
1:A:74:MET:HE2	1:A:96:ILE:CG1	2.37	0.54
1:B:53:TYR:O	1:B:54:GLN:HB2	2.07	0.54
1:B:1:MET:CG	1:B:2:THR:N	2.53	0.54
1:B:78:ASN:HA	1:B:102:TYR:HE2	1.73	0.53
1:A:38:PRO:CG	1:A:62:THR:OG1	2.54	0.53
1:A:218:ASN:HD21	1:A:220:LYS:HB2	1.73	0.53
1:A:11:LYS:HG3	1:A:12:ASP:N	2.17	0.53
1:A:19:GLU:HA	1:A:22:GLU:HB3	1.90	0.53
1:B:10:ARG:HB2	1:B:13:GLU:HG3	1.91	0.53
1:A:264:ASP:OD1	1:A:264:ASP:N	2.42	0.53
1:B:64:GLN:OE1	1:B:68:ASP:HB3	2.08	0.53
1:A:302:THR:HG21	1:B:143:GLU:CG	2.39	0.53
1:A:318:LEU:HD23	1:A:318:LEU:C	2.34	0.53
1:A:96:ILE:HG22	1:A:97:THR:N	2.23	0.53
1:B:54:GLN:HG2	1:B:56:LEU:N	2.22	0.53
1:A:283:LEU:HD12	1:A:283:LEU:C	2.33	0.53
1:B:10:ARG:NH1	1:B:53:TYR:HE2	2.06	0.53
1:B:85:ASP:O	1:B:89:ALA:HB2	2.09	0.53
1:A:108:ALA:HB3	1:A:160:VAL:CG1	2.38	0.53
1:A:210:VAL:HG13	1:A:211:PRO:HD2	1.90	0.53
1:A:213:ASN:HD21	2:A:401:NAI:C6A	2.21	0.53
1:A:302:THR:HG21	1:B:143:GLU:HG3	1.90	0.53
1:B:11:LYS:O	1:B:11:LYS:HG3	2.09	0.53
1:B:235:SER:HB2	2:B:401:NAI:C4D	2.38	0.53
1:A:135:ARG:HH11	1:A:135:ARG:CG	2.21	0.52
1:A:229:VAL:O	1:A:255:PHE:HB3	2.08	0.52
1:A:6:ALA:HB3	1:A:31:TYR:CB	2.35	0.52
1:A:38:PRO:N	1:A:62:THR:HG23	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:HG22	1:A:230:VAL:H	1.71	0.52
1:B:108:ALA:HB1	1:B:161:PHE:HB2	1.90	0.52
1:B:190:VAL:HG13	1:B:195:ASP:CB	2.39	0.52
1:A:18:ASN:O	1:A:22:GLU:CB	2.58	0.52
1:A:20:TRP:HE3	1:A:21:LYS:N	2.08	0.52
1:A:47:ALA:O	1:A:71:VAL:CG2	2.58	0.52
1:A:58:TYR:HB2	1:A:84:ILE:HG22	1.91	0.52
1:A:270:ASN:CA	1:B:134:LEU:O	2.57	0.52
1:A:270:ASN:N	1:B:134:LEU:O	2.41	0.52
1:B:17:LEU:HG	1:B:314:PHE:CZ	2.44	0.52
1:B:235:SER:HB2	2:B:401:NAI:H4D	1.92	0.52
1:A:318:LEU:O	1:A:318:LEU:CD2	2.57	0.52
1:B:36:LEU:HD12	1:B:36:LEU:C	2.32	0.52
1:A:9:ILE:CG2	1:A:31:TYR:HD2	2.19	0.52
1:B:96:ILE:HG22	1:B:97:THR:N	2.25	0.52
1:B:214:VAL:O	1:B:214:VAL:HG12	2.09	0.52
1:B:241:ASP:O	1:B:242:THR:C	2.53	0.52
1:B:266:VAL:O	1:B:266:VAL:CG1	2.58	0.52
1:B:173:ILE:HD11	1:B:199:GLN:HE21	1.74	0.52
1:B:176:ASP:OD1	2:B:401:NAI:H1B	2.09	0.52
1:A:180:ASN:ND2	1:A:183:LEU:HD22	2.25	0.52
1:B:5:PHE:HE2	1:B:7:TYR:CZ	2.28	0.52
1:B:9:ILE:CG2	1:B:31:TYR:CD2	2.85	0.52
1:A:210:VAL:CG1	1:A:212:ALA:HB3	2.40	0.52
1:B:125:MET:HE3	1:B:128:LYS:HE2	1.89	0.51
1:B:318:LEU:O	1:B:322:ASN:HB2	2.10	0.51
2:B:401:NAI:H42N	3:B:402:OXM:O1	2.08	0.51
1:A:20:TRP:O	1:A:20:TRP:CD2	2.63	0.51
1:A:297:HIS:NE2	2:A:401:NAI:C7N	2.73	0.51
1:B:43:LEU:C	1:B:45:LYS:H	2.17	0.51
1:B:86:MET:HB3	1:B:332:LEU:CG	2.35	0.51
1:B:88:LYS:C	1:B:92:LEU:HD12	2.35	0.51
1:A:43:LEU:C	1:A:45:LYS:N	2.68	0.51
1:A:108:ALA:CB	1:A:160:VAL:HG12	2.40	0.51
1:B:14:GLU:CB	1:B:15:PRO:CD	2.87	0.51
1:B:81:VAL:HG11	1:B:330:VAL:CG1	2.20	0.51
1:B:180:ASN:O	1:B:184:GLU:HB3	2.10	0.51
1:B:319:LYS:HD3	1:B:325:LYS:C	2.36	0.51
1:A:64:GLN:O	1:A:65:ALA:C	2.53	0.51
1:B:242:THR:HG22	1:B:246:ILE:HD12	1.92	0.51
1:B:40:THR:C	1:B:42:LYS:N	2.66	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:TYR:N	1:A:51:VAL:O	2.42	0.51
1:A:266:VAL:O	1:A:266:VAL:HG13	2.11	0.51
1:B:20:TRP:CE3	1:B:21:LYS:N	2.78	0.51
1:B:261:THR:HG23	1:B:265:GLU:OE1	2.11	0.51
1:A:12:ASP:O	1:A:16:PHE:CE2	2.64	0.51
1:B:79:VAL:HG13	1:B:80:GLY:N	2.25	0.51
1:B:142:ARG:HD2	1:B:147:GLN:NE2	2.25	0.51
1:B:314:PHE:O	1:B:315:ASN:O	2.28	0.51
1:A:90:LYS:C	1:A:92:LEU:N	2.67	0.51
1:A:269:PHE:HD1	1:B:134:LEU:HD23	1.76	0.51
1:A:9:ILE:HG22	1:A:9:ILE:O	2.10	0.51
1:A:17:LEU:HD23	1:A:18:ASN:HD22	1.76	0.51
1:A:58:TYR:HD2	1:A:84:ILE:HG23	1.74	0.51
1:A:153:GLY:HA3	1:A:206:HIS:O	2.11	0.51
1:A:270:ASN:O	1:A:270:ASN:CG	2.50	0.51
1:A:306:VAL:O	1:A:309:MET:HB2	2.11	0.51
1:B:27:ILE:HD11	1:B:318:LEU:HD11	1.93	0.51
1:B:210:VAL:O	1:B:213:ASN:N	2.44	0.51
1:A:59:THR:C	1:A:61:ASP:N	2.64	0.50
1:B:20:TRP:CE3	1:B:21:LYS:HA	2.47	0.50
1:B:48:ASP:HB3	1:B:321:ILE:CG1	2.41	0.50
1:B:85:ASP:O	1:B:89:ALA:CB	2.59	0.50
1:B:155:GLY:N	2:B:401:NAI:H51A	2.26	0.50
1:A:105:ASN:O	1:A:109:GLU:HB2	2.11	0.50
1:A:155:GLY:O	1:A:156:HIS:C	2.51	0.50
1:A:222:ILE:O	1:A:225:MET:HB2	2.11	0.50
1:A:329:PRO:O	1:A:332:LEU:HD23	2.12	0.50
1:B:21:LYS:HE3	1:B:24:HIS:O	2.10	0.50
1:B:48:ASP:HB3	1:B:321:ILE:HD11	1.93	0.50
1:A:21:LYS:O	1:A:21:LYS:NZ	2.39	0.50
1:A:131:LYS:O	1:A:132:ARG:CB	2.59	0.50
1:B:11:LYS:O	1:B:15:PRO:CD	2.59	0.50
1:A:149:VAL:CG2	1:A:165:MET:CE	2.81	0.50
1:B:40:THR:C	1:B:42:LYS:H	2.19	0.50
1:B:179:LYS:O	1:B:180:ASN:C	2.54	0.50
1:B:302:THR:HG22	1:B:305:ALA:H	1.76	0.50
1:B:314:PHE:O	1:B:315:ASN:C	2.55	0.50
1:A:305:ALA:O	1:A:308:ASN:HB2	2.12	0.50
1:B:175:TYR:CD2	1:B:193:LEU:HD13	2.46	0.50
1:A:37:THR:O	1:A:38:PRO:C	2.55	0.50
1:A:131:LYS:O	1:A:132:ARG:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:HE2	1:A:280:ASP:O	1.94	0.50
1:B:190:VAL:CG1	1:B:195:ASP:HB2	2.41	0.50
1:A:32:THR:CG2	1:A:33:ASP:N	2.75	0.50
1:A:35:LEU:HD13	1:A:54:GLN:HG2	1.94	0.50
1:A:105:ASN:HD22	1:B:145:ARG:NH2	2.08	0.50
1:A:31:TYR:HD1	1:A:31:TYR:N	2.06	0.50
1:B:28:ASP:OD1	1:B:30:ASP:OD1	2.29	0.50
1:A:110:HIS:O	1:A:114:GLN:HG2	2.11	0.49
1:A:193:LEU:HG	1:A:197:TYR:CZ	2.47	0.49
1:A:295:THR:HG22	1:A:296:PRO:CD	2.38	0.49
1:B:229:VAL:HG22	1:B:230:VAL:N	2.27	0.49
1:A:20:TRP:C	1:A:20:TRP:CD2	2.89	0.49
1:B:18:ASN:ND2	1:B:18:ASN:H	2.01	0.49
1:B:118:VAL:HG21	1:B:258:VAL:HG23	1.94	0.49
1:A:11:LYS:O	1:A:14:GLU:HB2	2.12	0.49
1:A:155:GLY:N	2:A:401:NAI:H52A	2.28	0.49
1:B:210:VAL:C	1:B:212:ALA:H	2.19	0.49
1:B:273:TRP:CH2	1:B:279:PRO:HG3	2.47	0.49
1:A:8:ALA:O	1:A:77:ARG:NH2	2.45	0.49
1:A:35:LEU:O	1:A:37:THR:HG23	2.13	0.49
1:A:82:ASP:OD1	1:A:82:ASP:O	2.31	0.49
1:A:318:LEU:C	1:A:318:LEU:CD2	2.85	0.49
1:A:74:MET:HE1	1:A:96:ILE:HD11	1.95	0.49
1:B:125:MET:CE	1:B:128:LYS:CE	2.89	0.49
1:A:99:VAL:O	1:A:99:VAL:CG1	2.58	0.49
1:A:190:VAL:CG1	1:A:191:ASP:N	2.75	0.49
1:A:269:PHE:CD1	1:B:134:LEU:HD23	2.46	0.49
1:B:90:LYS:C	1:B:93:GLY:H	2.21	0.49
1:A:135:ARG:NH2	1:B:272:ASP:HB2	2.27	0.49
1:B:9:ILE:O	1:B:9:ILE:HG23	2.13	0.49
1:B:154:THR:HG21	1:B:183:LEU:HD23	1.90	0.49
1:B:203:ILE:CD1	1:B:225:MET:HE2	2.42	0.49
1:B:308:ASN:O	1:B:312:LYS:N	2.45	0.49
1:A:198:LYS:HE3	1:A:198:LYS:HB2	1.61	0.49
1:B:327:ASP:O	1:B:328:SER:HB2	2.11	0.49
1:B:310:VAL:O	1:B:313:ALA:HB3	2.13	0.49
1:B:319:LYS:HB2	1:B:326:PRO:HB3	1.93	0.49
1:B:36:LEU:HD13	1:B:41:ALA:CA	2.43	0.48
1:A:144:VAL:C	1:A:146:ASP:H	2.21	0.48
1:A:237:GLY:H	1:A:261:THR:HG21	1.78	0.48
1:B:2:THR:HG22	1:B:3:LYS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:O	1:B:38:PRO:C	2.55	0.48
1:B:260:ASP:CG	1:B:298:THR:H	2.17	0.48
1:A:18:ASN:O	1:A:22:GLU:HB3	2.13	0.48
1:A:39:GLU:O	1:A:42:LYS:HG2	2.13	0.48
1:A:210:VAL:HG13	1:A:212:ALA:N	2.11	0.48
1:A:235:SER:CA	2:A:401:NAI:H1D	2.44	0.48
1:B:32:THR:HG22	1:B:34:LYS:O	2.13	0.48
1:A:20:TRP:C	1:A:20:TRP:HE3	2.20	0.48
1:A:142:ARG:HH11	1:A:147:GLN:NE2	2.11	0.48
1:A:278:PHE:CE2	1:A:280:ASP:O	2.66	0.48
1:A:328:SER:O	1:A:332:LEU:HD21	2.13	0.48
1:B:74:MET:O	1:B:96:ILE:HA	2.13	0.48
1:B:143:GLU:O	1:B:147:GLN:OE1	2.31	0.48
1:A:24:HIS:CE1	1:A:318:LEU:CD1	2.97	0.48
1:A:135:ARG:CG	1:A:135:ARG:NH1	2.77	0.48
1:A:144:VAL:C	1:A:146:ASP:N	2.72	0.48
1:B:173:ILE:HD11	1:B:199:GLN:CG	2.43	0.48
1:A:2:THR:HG22	1:A:321:ILE:HD13	1.96	0.48
1:A:5:PHE:HA	1:A:30:ASP:O	2.13	0.48
1:A:20:TRP:HZ3	1:A:29:VAL:HG21	1.77	0.48
1:A:109:GLU:OE1	1:B:143:GLU:HB3	2.14	0.48
1:A:217:ILE:HB	1:A:240:VAL:HG13	1.95	0.48
1:A:334:LYS:HA	1:A:334:LYS:HD3	1.63	0.48
1:B:207:VAL:HG22	1:B:208:PRO:HD2	1.94	0.48
1:A:2:THR:CG2	1:A:321:ILE:HD13	2.44	0.47
1:A:245:VAL:O	1:A:246:ILE:C	2.53	0.47
1:B:203:ILE:HD13	1:B:225:MET:HE2	1.96	0.47
1:A:74:MET:HE2	1:A:96:ILE:HG12	1.96	0.47
1:A:97:THR:CA	1:A:330:VAL:HG23	2.45	0.47
1:A:209:ASP:HB2	1:A:236:ARG:CB	2.43	0.47
1:B:5:PHE:HA	1:B:30:ASP:O	2.14	0.47
1:B:64:GLN:C	1:B:66:LEU:N	2.68	0.47
1:A:132:ARG:NH1	1:B:288:ASP:OD1	2.44	0.47
1:A:136:TRP:NE1	1:B:270:ASN:ND2	2.62	0.47
1:B:45:LYS:HA	1:B:69:ALA:HB1	1.96	0.47
1:B:75:SER:OG	1:B:97:THR:CB	2.62	0.47
1:B:120:ARG:O	1:B:121:GLN:HB2	2.14	0.47
1:A:129:MET:SD	1:B:296:PRO:HG3	2.55	0.47
1:B:2:THR:CG2	1:B:3:LYS:N	2.76	0.47
1:B:124:ARG:O	1:B:128:LYS:HG3	2.15	0.47
1:B:316:ASN:HD21	1:B:327:ASP:CB	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ARG:HH21	1:B:306:VAL:CG1	2.27	0.47
1:A:11:LYS:HZ2	1:A:14:GLU:CD	2.22	0.47
1:A:105:ASN:ND2	1:B:145:ARG:NH2	2.63	0.47
1:B:6:ALA:N	1:B:30:ASP:O	2.44	0.47
1:B:7:TYR:HB2	1:B:52:VAL:HB	1.97	0.47
1:B:88:LYS:O	1:B:92:LEU:HD12	2.15	0.47
1:A:19:GLU:CA	1:A:22:GLU:HB3	2.44	0.47
1:A:151:VAL:HG23	1:A:173:ILE:O	2.15	0.47
1:A:157:ILE:CD1	2:A:401:NAI:H51N	2.21	0.47
1:A:270:ASN:HA	1:B:134:LEU:C	2.39	0.47
1:B:90:LYS:HD2	1:B:90:LYS:HA	1.26	0.47
1:B:125:MET:O	1:B:128:LYS:HB2	2.15	0.47
1:B:180:ASN:C	1:B:180:ASN:OD1	2.58	0.47
1:A:37:THR:C	1:A:39:GLU:N	2.72	0.47
1:A:232:VAL:HG22	1:A:258:VAL:HB	1.96	0.47
1:B:251:SER:OG	1:B:252:GLY:N	2.47	0.47
1:A:235:SER:HA	2:A:401:NAI:H2N	1.96	0.47
1:B:32:THR:CG2	1:B:34:LYS:O	2.62	0.47
1:B:43:LEU:HD12	1:B:43:LEU:O	2.14	0.47
1:B:154:THR:HG23	1:B:159:GLN:CG	2.45	0.47
1:A:219:ASP:CG	1:A:247:ARG:HH12	2.23	0.47
1:B:1:MET:CG	1:B:2:THR:H	2.16	0.47
1:B:61:ASP:O	1:B:62:THR:C	2.57	0.47
1:B:86:MET:O	1:B:89:ALA:HB3	2.15	0.47
1:A:142:ARG:NH1	1:A:147:GLN:HE21	2.11	0.46
1:A:267:GLY:O	1:A:271:LYS:HD3	2.16	0.46
1:B:9:ILE:CG2	1:B:31:TYR:HD2	2.27	0.46
1:B:37:THR:HB	1:B:38:PRO:HD2	1.97	0.46
1:B:38:PRO:HG3	1:B:62:THR:HA	1.97	0.46
1:B:149:VAL:HG22	1:B:202:VAL:HB	1.97	0.46
1:A:59:THR:O	1:A:63:LEU:CD1	2.60	0.46
1:A:113:ILE:HD13	1:B:116:ALA:HB3	1.97	0.46
1:A:136:TRP:HE1	1:B:270:ASN:ND2	2.13	0.46
1:A:259:MET:HB2	1:A:259:MET:HE3	1.60	0.46
1:B:7:TYR:HE1	1:B:40:THR:HG22	1.79	0.46
1:B:42:LYS:NZ	1:B:42:LYS:CB	2.78	0.46
1:B:86:MET:O	1:B:332:LEU:CD1	2.63	0.46
1:B:151:VAL:HG21	1:B:162:MET:CE	2.42	0.46
1:A:103:SER:HA	1:A:104:PRO:HD2	1.85	0.46
1:A:107:ILE:HG23	1:A:299:ALA:HB1	1.97	0.46
1:A:267:GLY:HA2	1:A:271:LYS:HZ1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TRP:HE3	1:B:21:LYS:CA	2.29	0.46
1:B:129:MET:O	1:B:132:ARG:HD2	2.15	0.46
1:B:222:ILE:HD13	1:B:222:ILE:HG23	1.69	0.46
1:B:231:ILE:O	1:B:257:PHE:HA	2.16	0.46
1:A:6:ALA:HB1	1:A:9:ILE:HD11	1.93	0.46
1:A:102:TYR:CE2	1:A:309:MET:SD	3.08	0.46
1:A:193:LEU:HG	1:A:197:TYR:CE1	2.50	0.46
1:A:228:GLY:CA	1:A:255:PHE:HB2	2.45	0.46
1:B:17:LEU:HD21	1:B:29:VAL:HG11	1.98	0.46
1:B:135:ARG:HH11	1:B:135:ARG:CG	2.29	0.46
1:B:90:LYS:CB	1:B:332:LEU:CD1	2.86	0.46
1:A:71:VAL:HG12	1:A:73:LYS:H	1.79	0.46
1:A:308:ASN:O	1:A:309:MET:C	2.59	0.46
1:B:218:ASN:HD22	1:B:220:LYS:H	1.52	0.46
1:A:59:THR:O	1:A:61:ASP:N	2.49	0.46
1:A:62:THR:HA	1:A:65:ALA:CB	2.46	0.46
1:B:5:PHE:HB2	1:B:47:ALA:CB	2.46	0.46
1:B:96:ILE:HG22	1:B:97:THR:H	1.80	0.46
1:A:132:ARG:NH2	1:B:284:ALA:HB1	2.30	0.46
1:A:182:GLU:C	1:A:182:GLU:OE1	2.59	0.46
1:A:185:LYS:HD2	1:A:185:LYS:HA	1.28	0.46
1:B:102:TYR:HD2	1:B:309:MET:CG	2.22	0.46
1:A:123:LYS:HE2	1:A:289:ARG:O	2.16	0.45
1:A:143:GLU:OE1	1:A:145:ARG:HD2	2.16	0.45
1:A:182:GLU:OE1	1:A:183:LEU:HD12	2.15	0.45
1:B:164:ILE:O	1:B:168:PHE:HD2	1.98	0.45
1:A:162:MET:HB3	1:A:163:ARG:NH1	2.31	0.45
1:A:263:GLU:C	1:A:265:GLU:H	2.23	0.45
1:B:207:VAL:CG2	2:B:401:NAI:C4A	2.94	0.45
1:A:156:HIS:CD2	2:A:401:NAI:O2N	2.69	0.45
1:A:277:GLU:O	1:A:279:PRO:HD3	2.16	0.45
1:A:97:THR:OG1	1:A:320:LEU:HD21	2.17	0.45
1:A:128:LYS:HB3	1:A:133:ASP:HB3	1.98	0.45
1:A:139:THR:O	1:A:139:THR:CG2	2.52	0.45
1:A:152:VAL:HB	1:A:205:LEU:HD12	1.98	0.45
1:B:61:ASP:C	1:B:63:LEU:N	2.73	0.45
1:B:90:LYS:C	1:B:92:LEU:N	2.70	0.45
1:A:61:ASP:OD1	1:A:62:THR:N	2.49	0.45
1:A:31:TYR:HB2	1:A:32:THR:H	1.61	0.45
1:A:49:GLY:HA3	1:A:317:ASN:HD21	1.82	0.45
1:A:60:ALA:HB1	1:A:88:LYS:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:HG12	1:A:213:ASN:N	2.23	0.45
1:A:180:ASN:HA	1:A:181:PRO:HD2	1.69	0.45
1:A:237:GLY:N	1:A:261:THR:HG21	2.32	0.45
1:B:86:MET:CE	1:B:332:LEU:CB	2.93	0.45
1:B:282:ARG:HG3	1:B:283:LEU:H	1.81	0.45
1:A:278:PHE:CD2	1:A:284:ALA:HB2	2.50	0.45
1:B:17:LEU:HB3	1:B:18:ASN:HD21	1.80	0.45
1:B:85:ASP:O	1:B:89:ALA:N	2.44	0.45
1:B:255:PHE:O	1:B:291:ASN:ND2	2.47	0.45
1:A:300:PHE:CG	1:A:301:TYR:N	2.84	0.44
1:B:20:TRP:CE3	1:B:21:LYS:CA	3.00	0.44
1:B:154:THR:HG23	1:B:159:GLN:HG2	1.98	0.44
1:B:143:GLU:OE1	1:B:145:ARG:HD2	2.18	0.44
1:B:280:ASP:OD1	1:B:280:ASP:C	2.60	0.44
1:B:287:ILE:HA	1:B:294:VAL:HG23	1.97	0.44
1:B:21:LYS:CE	1:B:24:HIS:O	2.65	0.44
1:B:77:ARG:O	1:B:309:MET:HG2	2.17	0.44
1:B:302:THR:CG2	1:B:304:HIS:H	2.30	0.44
1:A:9:ILE:HD12	1:A:77:ARG:CZ	2.43	0.44
1:A:298:THR:O	1:A:299:ALA:C	2.61	0.44
1:A:15:PRO:O	1:A:18:ASN:HB2	2.17	0.44
1:A:149:VAL:HG11	1:A:165:MET:HE3	1.99	0.44
1:A:168:PHE:CE2	1:B:109:GLU:HG2	2.53	0.44
1:A:207:VAL:HA	1:A:208:PRO:HD3	1.89	0.44
1:B:78:ASN:OD1	1:B:78:ASN:N	2.51	0.44
1:B:180:ASN:HA	1:B:181:PRO:HD3	1.80	0.44
1:A:7:TYR:CD2	1:A:36:LEU:CD1	2.94	0.44
1:A:331:ALA:C	1:A:333:ASN:N	2.75	0.44
1:B:47:ALA:O	1:B:71:VAL:HG21	2.17	0.44
1:A:89:ALA:O	1:A:94:PHE:HB2	2.18	0.44
1:A:128:LYS:HE3	1:A:135:ARG:O	2.18	0.44
1:A:190:VAL:HG12	1:A:192:SER:H	1.82	0.44
1:A:302:THR:CG2	1:B:143:GLU:HG3	2.47	0.44
1:B:297:HIS:HE2	2:B:401:NAI:H42N	1.82	0.44
1:B:319:LYS:CE	1:B:325:LYS:O	2.66	0.44
1:A:59:THR:C	1:A:61:ASP:H	2.26	0.44
1:A:168:PHE:HE2	1:B:109:GLU:HG2	1.83	0.44
1:A:238:ARG:H	1:A:238:ARG:HG2	1.40	0.44
1:B:13:GLU:O	1:B:14:GLU:C	2.61	0.44
1:B:184:GLU:HA	1:B:189:TYR:CD1	2.49	0.44
1:B:243:ASP:O	1:B:244:ALA:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:OG1	1:A:40:THR:OG1	1.69	0.44
1:A:113:ILE:HD11	1:B:116:ALA:CB	2.38	0.44
1:A:282:ARG:HH11	1:A:282:ARG:HD3	1.43	0.44
1:B:10:ARG:HH11	1:B:53:TYR:HE2	1.65	0.44
1:B:268:VAL:HG11	1:B:283:LEU:HD23	1.98	0.44
1:A:140:ILE:HG13	1:B:301:TYR:CE1	2.53	0.43
1:B:64:GLN:CA	1:B:67:ALA:HB3	2.42	0.43
1:B:134:LEU:N	1:B:134:LEU:HD12	2.33	0.43
1:B:270:ASN:O	1:B:271:LYS:HD3	2.18	0.43
1:B:278:PHE:CD2	1:B:284:ALA:HB2	2.52	0.43
1:B:5:PHE:CE2	1:B:7:TYR:CZ	3.06	0.43
1:B:193:LEU:HD12	1:B:193:LEU:HA	1.71	0.43
1:A:2:THR:CG2	1:A:27:ILE:HG23	2.48	0.43
1:A:20:TRP:O	1:A:24:HIS:HB2	2.18	0.43
1:A:237:GLY:H	1:A:261:THR:CG2	2.31	0.43
1:A:38:PRO:N	1:A:62:THR:CG2	2.81	0.43
1:A:64:GLN:O	1:A:68:ASP:OD1	2.37	0.43
1:A:96:ILE:CB	1:A:330:VAL:HG21	2.42	0.43
1:A:315:ASN:O	1:A:316:ASN:C	2.61	0.43
1:A:316:ASN:ND2	1:A:327:ASP:O	2.52	0.43
1:B:9:ILE:HG21	1:B:31:TYR:HD2	1.68	0.43
1:A:59:THR:O	1:A:60:ALA:C	2.61	0.43
1:A:105:ASN:ND2	1:B:145:ARG:CZ	2.81	0.43
1:B:158:GLY:O	1:B:162:MET:HG3	2.19	0.43
1:B:235:SER:HB2	2:B:401:NAI:H1D	2.00	0.43
1:B:317:ASN:O	1:B:320:LEU:CB	2.65	0.43
1:A:159:GLN:O	1:A:163:ARG:HD2	2.18	0.43
1:A:163:ARG:O	1:A:166:GLU:HB2	2.18	0.43
1:B:9:ILE:O	1:B:9:ILE:HG22	2.16	0.43
1:B:10:ARG:HH12	1:B:309:MET:HE1	1.83	0.43
1:B:21:LYS:O	1:B:23:ALA:N	2.51	0.43
1:B:36:LEU:CD1	1:B:41:ALA:HB2	2.43	0.43
1:A:156:HIS:CD2	1:A:156:HIS:N	2.86	0.43
1:A:177:ILE:HA	1:A:177:ILE:HD12	1.63	0.43
1:B:53:TYR:O	1:B:54:GLN:CB	2.67	0.43
1:B:64:GLN:O	1:B:65:ALA:C	2.60	0.43
1:B:173:ILE:CD1	1:B:199:GLN:CG	2.97	0.43
1:B:177:ILE:HD13	2:B:401:NAI:C2A	2.49	0.43
1:A:237:GLY:N	1:A:261:THR:CG2	2.82	0.43
1:A:281:LYS:O	1:A:282:ARG:C	2.61	0.43
1:B:262:TYR:O	1:B:265:GLU:CB	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:SER:N	1:B:329:PRO:CD	2.82	0.43
1:A:190:VAL:HG12	1:A:192:SER:N	2.33	0.43
1:B:240:VAL:HG12	1:B:241:ASP:H	1.84	0.43
1:B:261:THR:HG22	1:B:262:TYR:N	2.34	0.43
1:A:184:GLU:HB3	1:A:189:TYR:CD2	2.54	0.42
1:B:1:MET:HE2	1:B:1:MET:HB2	1.72	0.42
1:B:65:ALA:O	1:B:68:ASP:OD1	2.37	0.42
1:B:122:ASP:O	1:B:125:MET:N	2.52	0.42
1:B:125:MET:CE	1:B:128:LYS:HE3	2.43	0.42
1:B:210:VAL:HB	1:B:213:ASN:HD22	1.84	0.42
1:A:155:GLY:N	2:A:401:NAI:C5B	2.83	0.42
1:A:228:GLY:C	1:A:255:PHE:HB2	2.43	0.42
1:A:267:GLY:HA2	1:A:271:LYS:NZ	2.34	0.42
1:A:302:THR:O	1:A:303:THR:C	2.61	0.42
1:B:20:TRP:CE3	1:B:20:TRP:C	2.97	0.42
1:B:32:THR:HG23	1:B:34:LYS:H	1.83	0.42
1:B:61:ASP:O	1:B:63:LEU:N	2.53	0.42
1:B:173:ILE:O	1:B:173:ILE:HG22	2.14	0.42
1:A:315:ASN:O	1:A:317:ASN:N	2.52	0.42
1:A:331:ALA:H	1:A:332:LEU:HG	1.84	0.42
1:B:48:ASP:O	1:B:71:VAL:HG13	2.18	0.42
1:B:234:CYS:O	2:B:401:NAI:N7N	2.52	0.42
1:B:302:THR:HG23	1:B:304:HIS:H	1.83	0.42
1:A:58:TYR:CD2	1:A:84:ILE:HG22	2.54	0.42
1:A:288:ASP:O	1:A:289:ARG:C	2.61	0.42
1:B:135:ARG:CG	1:B:135:ARG:NH1	2.81	0.42
1:B:241:ASP:OD2	1:B:244:ALA:HB2	2.20	0.42
1:A:287:ILE:HD13	1:A:287:ILE:HG21	1.74	0.42
1:B:183:LEU:N	1:B:183:LEU:HD13	2.35	0.42
2:B:401:NAI:C5N	3:B:402:OXM:HN2	1.92	0.42
1:A:4:VAL:HG13	1:A:317:ASN:ND2	2.33	0.42
1:A:208:PRO:HG2	2:A:401:NAI:H8A	2.01	0.42
1:B:316:ASN:HD21	1:B:327:ASP:CA	2.32	0.42
1:A:17:LEU:HD23	1:A:17:LEU:C	2.44	0.42
1:A:20:TRP:CE3	1:A:21:LYS:HA	2.55	0.42
1:A:32:THR:HG23	1:A:33:ASP:H	1.84	0.42
1:A:55:GLN:O	1:A:55:GLN:HG2	2.20	0.42
1:B:20:TRP:CZ3	1:B:29:VAL:HG21	2.55	0.42
1:B:63:LEU:O	1:B:64:GLN:C	2.61	0.42
1:B:235:SER:HA	2:B:401:NAI:H2N	2.01	0.42
1:A:7:TYR:CD2	1:A:36:LEU:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:HG23	1:A:329:PRO:HA	2.01	0.42
1:A:103:SER:HB2	1:B:145:ARG:HH12	1.85	0.42
1:A:210:VAL:CG1	1:A:211:PRO:HD2	2.49	0.42
1:A:317:ASN:O	1:A:319:LYS:N	2.53	0.42
1:B:175:TYR:CD2	1:B:175:TYR:C	2.98	0.42
1:A:85:ASP:O	1:A:89:ALA:CB	2.57	0.42
1:B:40:THR:O	1:B:43:LEU:N	2.50	0.42
1:B:154:THR:H	2:B:401:NAI:H4B	1.84	0.42
1:B:293:LEU:HD12	1:B:293:LEU:HA	1.91	0.42
1:A:88:LYS:O	1:A:92:LEU:HB2	2.19	0.41
1:A:217:ILE:CG2	1:A:240:VAL:HG12	2.50	0.41
1:B:197:TYR:N	1:B:197:TYR:CD1	2.87	0.41
1:B:213:ASN:O	1:B:215:HIS:N	2.52	0.41
1:A:66:LEU:HD23	1:A:94:PHE:CZ	2.55	0.41
1:B:77:ARG:HG3	1:B:313:ALA:HB2	2.02	0.41
1:B:282:ARG:HG3	1:B:283:LEU:N	2.36	0.41
1:A:7:TYR:O	1:A:8:ALA:HB3	2.20	0.41
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.56	0.41
1:A:71:VAL:HG12	1:A:73:LYS:N	2.35	0.41
1:A:86:MET:HE1	1:A:330:VAL:HG11	2.02	0.41
1:B:319:LYS:HD3	1:B:325:LYS:O	2.20	0.41
1:A:144:VAL:H	1:A:144:VAL:HG23	1.68	0.41
1:A:209:ASP:HB2	1:A:236:ARG:HB3	2.02	0.41
1:A:268:VAL:HG11	1:A:283:LEU:HD23	2.03	0.41
1:A:306:VAL:HG21	1:B:140:ILE:CD1	2.51	0.41
1:B:5:PHE:CD2	1:B:7:TYR:CE2	3.09	0.41
1:A:39:GLU:HG3	1:A:40:THR:N	2.33	0.41
1:A:260:ASP:OD2	1:A:298:THR:N	2.33	0.41
1:A:300:PHE:CD1	1:A:301:TYR:N	2.88	0.41
1:A:5:PHE:O	1:A:50:VAL:CG1	2.48	0.41
1:A:7:TYR:CE1	1:A:36:LEU:CD1	3.02	0.41
1:A:38:PRO:HA	1:A:62:THR:CG2	2.19	0.41
1:A:90:LYS:O	1:A:91:GLU:C	2.63	0.41
1:A:144:VAL:O	1:A:145:ARG:C	2.61	0.41
1:A:182:GLU:OE1	1:A:183:LEU:N	2.53	0.41
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.78	0.41
1:A:281:LYS:HE3	1:A:281:LYS:HB3	1.63	0.41
1:B:66:LEU:O	1:B:67:ALA:C	2.63	0.41
1:B:262:TYR:CE2	1:B:283:LEU:HB2	2.55	0.41
1:B:21:LYS:C	1:B:23:ALA:N	2.76	0.41
1:B:90:LYS:HD2	1:B:90:LYS:C	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASP:O	1:B:177:ILE:C	2.63	0.41
1:B:242:THR:O	1:B:246:ILE:HD12	2.21	0.41
1:A:266:VAL:O	1:A:266:VAL:CG1	2.68	0.41
1:B:319:LYS:HD3	1:B:326:PRO:CA	2.50	0.41
1:A:21:LYS:HZ1	1:A:24:HIS:C	2.27	0.41
1:A:96:ILE:HG21	1:A:330:VAL:HG21	1.82	0.41
1:A:98:ASN:OD1	1:A:332:LEU:HD13	2.20	0.41
1:B:10:ARG:NH2	1:B:13:GLU:HG2	2.36	0.41
1:B:32:THR:HG23	1:B:34:LYS:N	2.36	0.41
1:B:178:PHE:O	1:B:180:ASN:N	2.53	0.41
1:B:183:LEU:N	1:B:183:LEU:CD1	2.84	0.41
1:B:262:TYR:HB3	1:B:265:GLU:CB	2.40	0.41
1:B:335:ASN:ND2	1:B:335:ASN:O	2.54	0.41
1:A:49:GLY:HA3	1:A:73:LYS:HB3	2.03	0.41
1:B:177:ILE:HA	1:B:177:ILE:HD12	1.69	0.41
1:B:282:ARG:O	1:B:285:ASP:N	2.54	0.41
1:A:64:GLN:C	1:A:66:LEU:N	2.76	0.40
1:A:74:MET:CE	1:A:96:ILE:HD13	2.47	0.40
1:A:209:ASP:OD2	1:A:238:ARG:HG3	2.21	0.40
1:A:260:ASP:OD2	1:A:295:THR:HB	2.21	0.40
1:B:7:TYR:HE1	1:B:40:THR:CG2	2.34	0.40
1:B:214:VAL:O	1:B:215:HIS:CB	2.68	0.40
1:B:261:THR:OG1	1:B:297:HIS:CE1	2.74	0.40
1:B:273:TRP:CZ3	1:B:279:PRO:CG	2.98	0.40
1:A:11:LYS:O	1:A:11:LYS:HE3	2.21	0.40
1:A:262:TYR:CE2	1:A:283:LEU:HB2	2.56	0.40
1:B:6:ALA:O	1:B:31:TYR:HA	2.21	0.40
1:B:40:THR:O	1:B:41:ALA:C	2.64	0.40
1:A:24:HIS:ND1	1:A:318:LEU:HD12	2.37	0.40
1:A:25:LYS:NZ	1:A:25:LYS:O	2.54	0.40
1:A:71:VAL:CG1	1:A:73:LYS:H	2.33	0.40
1:B:17:LEU:HD21	1:B:29:VAL:CG1	2.52	0.40
1:B:37:THR:C	1:B:39:GLU:N	2.74	0.40
1:B:307:ARG:O	1:B:311:VAL:HB	2.22	0.40
1:A:52:VAL:HG22	1:A:58:TYR:OH	2.21	0.40
1:A:178:PHE:O	1:A:180:ASN:N	2.55	0.40
1:A:217:ILE:HA	1:A:221:SER:OG	2.21	0.40
1:A:218:ASN:O	1:A:219:ASP:C	2.65	0.40
1:B:261:THR:CG2	1:B:265:GLU:OE1	2.69	0.40
1:B:331:ALA:O	1:B:333:ASN:N	2.55	0.40
1:B:233:ASN:ND2	1:B:240:VAL:HG23	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:TYR:O	1:B:265:GLU:CG	2.70	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	335/337 (99%)	263 (78%)	59 (18%)	13 (4%)	2	5
1	B	335/337 (99%)	271 (81%)	44 (13%)	20 (6%)	1	2
All	All	670/674 (99%)	534 (80%)	103 (15%)	33 (5%)	1	3

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	LEU
1	A	179	LYS
1	A	332	LEU
1	B	24	HIS
1	B	41	ALA
1	B	60	ALA
1	B	179	LYS
1	B	214	VAL
1	B	215	HIS
1	B	315	ASN
1	A	25	LYS
1	A	139	THR
1	A	145	ARG
1	A	215	HIS
1	A	310	VAL
1	A	331	ALA
1	B	156	HIS

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Mol	Chain	Res	Type
1	B	197	TYR
1	B	225	MET
1	B	238	ARG
1	B	316	ASN
1	B	328	SER
1	B	332	LEU
1	A	44	ALA
1	A	103	SER
1	B	132	ARG
1	A	309	MET
1	B	62	THR
1	B	103	SER
1	B	334	LYS
1	A	181	PRO
1	B	177	ILE
1	B	211	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	286/286 (100%)	196 (68%)	90 (32%)	0	1
1	B	286/286 (100%)	202 (71%)	84 (29%)	0	1
All	All	572/572 (100%)	398 (70%)	174 (30%)	0	1

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	9	ILE
1	A	11	LYS
1	A	12	ASP
1	A	17	LEU
1	A	20	TRP
1	A	21	LYS

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Mol	Chain	Res	Type
1	A	25	LYS
1	A	27	ILE
1	A	30	ASP
1	A	31	TYR
1	A	32	THR
1	A	33	ASP
1	A	35	LEU
1	A	36	LEU
1	A	39	GLU
1	A	40	THR
1	A	48	ASP
1	A	51	VAL
1	A	52	VAL
1	A	56	LEU
1	A	59	THR
1	A	72	THR
1	A	77	ARG
1	A	79	VAL
1	A	82	ASP
1	A	84	ILE
1	A	87	ASP
1	A	88	LYS
1	A	91	GLU
1	A	92	LEU
1	A	94	PHE
1	A	97	THR
1	A	98	ASN
1	A	99	VAL
1	A	102	TYR
1	A	109	GLU
1	A	132	ARG
1	A	134	LEU
1	A	135	ARG
1	A	138	PRO
1	A	142	ARG
1	A	145	ARG
1	A	151	VAL
1	A	156	HIS
1	A	163	ARG
1	A	166	GLU
1	A	173	ILE
1	A	177	ILE

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Mol	Chain	Res	Type
1	A	179	LYS
1	A	182	GLU
1	A	183	LEU
1	A	185	LYS
1	A	186	LYS
1	A	190	VAL
1	A	196	LEU
1	A	198	LYS
1	A	199	GLN
1	A	205	LEU
1	A	210	VAL
1	A	217	ILE
1	A	219	ASP
1	A	225	MET
1	A	229	VAL
1	A	238	ARG
1	A	240	VAL
1	A	246	ILE
1	A	259	MET
1	A	264	ASP
1	A	271	LYS
1	A	276	LYS
1	A	277	GLU
1	A	282	ARG
1	A	283	LEU
1	A	289	ARG
1	A	293	LEU
1	A	295	THR
1	A	297	HIS
1	A	298	THR
1	A	302	THR
1	A	303	THR
1	A	307	ARG
1	A	319	LYS
1	A	320	LEU
1	A	321	ILE
1	A	325	LYS
1	A	328	SER
1	A	330	VAL
1	A	332	LEU
1	A	335	ASN
1	B	1	MET

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Mol	Chain	Res	Type
1	B	3	LYS
1	B	9	ILE
1	B	11	LYS
1	B	17	LEU
1	B	18	ASN
1	B	21	LYS
1	B	22	GLU
1	B	27	ILE
1	B	32	THR
1	B	35	LEU
1	B	36	LEU
1	B	39	GLU
1	B	40	THR
1	B	42	LYS
1	B	43	LEU
1	B	48	ASP
1	B	52	VAL
1	B	56	LEU
1	B	57	ASP
1	B	61	ASP
1	B	63	LEU
1	B	71	VAL
1	B	74	MET
1	B	81	VAL
1	B	82	ASP
1	B	84	ILE
1	B	90	LYS
1	B	91	GLU
1	B	94	PHE
1	B	95	GLN
1	B	96	ILE
1	B	97	THR
1	B	98	ASN
1	B	99	VAL
1	B	101	VAL
1	B	102	TYR
1	B	107	ILE
1	B	126	ASP
1	B	140	ILE
1	B	145	ARG
1	B	147	GLN
1	B	151	VAL

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Mol	Chain	Res	Type
1	B	156	HIS
1	B	163	ARG
1	B	172	VAL
1	B	173	ILE
1	B	177	ILE
1	B	179	LYS
1	B	182	GLU
1	B	183	LEU
1	B	184	GLU
1	B	185	LYS
1	B	190	VAL
1	B	198	LYS
1	B	202	VAL
1	B	205	LEU
1	B	217	ILE
1	B	218	ASN
1	B	219	ASP
1	B	222	ILE
1	B	224	GLU
1	B	225	MET
1	B	246	ILE
1	B	258	VAL
1	B	266	VAL
1	B	271	LYS
1	B	277	GLU
1	B	281	LYS
1	B	289	ARG
1	B	293	LEU
1	B	295	THR
1	B	297	HIS
1	B	298	THR
1	B	302	THR
1	B	307	ARG
1	B	318	LEU
1	B	320	LEU
1	B	321	ILE
1	B	327	ASP
1	B	332	LEU
1	B	333	ASN
1	B	334	LYS
1	B	336	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	55	GLN
1	A	105	ASN
1	A	147	GLN
1	A	156	HIS
1	A	199	GLN
1	A	213	ASN
1	A	218	ASN
1	A	270	ASN
1	A	308	ASN
1	A	317	ASN
1	B	18	ASN
1	B	24	HIS
1	B	54	GLN
1	B	55	GLN
1	B	98	ASN
1	B	105	ASN
1	B	110	HIS
1	B	147	GLN
1	B	156	HIS
1	B	199	GLN
1	B	213	ASN
1	B	218	ASN
1	B	270	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	B	401	3	47,48,48	2.50	17 (36%)	64,73,73	2.21	20 (31%)
2	NAI	A	401	-	47,48,48	2.34	19 (40%)	64,73,73	2.62	26 (40%)
3	OXM	B	402	2	5,5,5	6.34	2 (40%)	2,6,6	2.76	1 (50%)
3	OXM	A	402	-	5,5,5	6.45	1 (20%)	2,6,6	3.92	1 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	B	401	3	-	16/29/72/72	0/5/5/5
2	NAI	A	401	-	1/1/13/16	10/29/72/72	0/5/5/5
3	OXM	B	402	2	-	3/4/4/4	-
3	OXM	A	402	-	-	3/4/4/4	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	OXM	C1-C2	-14.19	1.38	1.55
3	B	402	OXM	C1-C2	-13.96	1.38	1.55
2	B	401	NAI	PN-O3	8.22	1.68	1.59
2	A	401	NAI	PN-O3	7.54	1.67	1.59
2	B	401	NAI	O4D-C4D	5.57	1.57	1.45
2	B	401	NAI	C4N-C3N	-5.02	1.40	1.50
2	A	401	NAI	O2B-C2B	-4.60	1.31	1.43
2	A	401	NAI	C4N-C3N	-4.55	1.41	1.50
2	A	401	NAI	C7N-C3N	4.39	1.58	1.48
2	B	401	NAI	C7N-C3N	4.32	1.58	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAI	O4B-C4B	4.30	1.54	1.45
2	B	401	NAI	C2A-N3A	3.56	1.40	1.33
2	A	401	NAI	C1D-N1N	3.38	1.55	1.46
2	B	401	NAI	O3B-C3B	3.32	1.51	1.43
2	A	401	NAI	C4A-N9A	3.24	1.44	1.37
2	B	401	NAI	C5A-N7A	-3.21	1.33	1.39
2	B	401	NAI	PA-O3	-3.20	1.56	1.59
2	A	401	NAI	C4A-N3A	3.05	1.40	1.34
2	A	401	NAI	C2A-N3A	3.02	1.39	1.33
2	A	401	NAI	C5A-N7A	-3.02	1.33	1.39
2	B	401	NAI	O2B-C2B	-3.00	1.35	1.43
2	A	401	NAI	O4B-C4B	2.96	1.51	1.45
2	B	401	NAI	O2D-C2D	-2.90	1.35	1.43
2	B	401	NAI	C4A-N3A	2.73	1.39	1.34
2	A	401	NAI	O4D-C4D	2.67	1.50	1.45
2	B	401	NAI	C1D-N1N	2.67	1.53	1.46
2	B	401	NAI	C4A-N9A	2.44	1.42	1.37
2	A	401	NAI	C2B-C1B	-2.41	1.45	1.53
2	A	401	NAI	C5A-C6A	2.39	1.47	1.41
2	A	401	NAI	C4N-C5N	-2.38	1.42	1.49
2	A	401	NAI	O2D-C2D	-2.32	1.37	1.43
2	B	401	NAI	C4N-C5N	-2.31	1.43	1.49
2	B	401	NAI	C5A-C6A	2.31	1.47	1.41
2	A	401	NAI	C1B-N9A	-2.31	1.40	1.46
2	A	401	NAI	PA-O3	-2.24	1.57	1.59
2	A	401	NAI	O4D-C1D	2.19	1.47	1.42
2	A	401	NAI	C3D-C4D	2.16	1.58	1.53
3	B	402	OXM	O3-C2	-2.08	1.24	1.30
2	B	401	NAI	O3D-C3D	-2.02	1.38	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAI	C2B-C1B-N9A	7.06	130.86	113.30
2	A	401	NAI	C3N-C2N-N1N	-6.84	113.16	123.20
2	B	401	NAI	C3N-C2N-N1N	-6.38	113.83	123.20
2	A	401	NAI	C4A-N9A-C8A	-6.29	99.13	105.74
2	A	401	NAI	C2A-N1A-C6A	5.33	127.48	118.73
3	A	402	OXM	O3-C2-O2	-5.32	111.23	123.90
2	A	401	NAI	O2B-C2B-C3B	5.12	128.22	111.82
2	B	401	NAI	C2A-N1A-C6A	5.03	126.99	118.73
2	A	401	NAI	C6N-N1N-C2N	5.02	124.69	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAI	C1D-N1N-C2N	-4.99	112.91	121.14
2	B	401	NAI	C4A-N9A-C8A	-4.48	101.03	105.74
2	B	401	NAI	C1D-N1N-C2N	-4.40	113.89	121.14
2	A	401	NAI	O2B-C2B-C1B	4.40	125.26	110.10
2	B	401	NAI	C2D-C3D-C4D	4.09	110.51	102.61
2	A	401	NAI	N3A-C2A-N1A	-4.02	122.50	128.58
2	A	401	NAI	O4B-C1B-C2B	4.01	115.19	106.62
2	A	401	NAI	C2D-C3D-C4D	3.84	110.03	102.61
2	B	401	NAI	C2D-C1D-N1N	3.77	122.59	113.31
2	B	401	NAI	N3A-C2A-N1A	-3.76	122.89	128.58
3	B	402	OXM	O3-C2-O2	-3.54	115.48	123.90
2	B	401	NAI	C6N-N1N-C2N	3.43	122.99	119.32
2	B	401	NAI	C2B-C3B-C4B	3.30	108.99	102.61
2	B	401	NAI	O4D-C1D-N1N	3.28	114.34	108.08
2	A	401	NAI	C2D-C1D-N1N	3.16	121.08	113.31
2	B	401	NAI	O3D-C3D-C2D	3.02	121.49	111.82
2	B	401	NAI	C4B-O4B-C1B	-2.95	102.95	109.47
2	B	401	NAI	O2B-C2B-C3B	2.93	121.19	111.82
2	B	401	NAI	O2D-C2D-C3D	2.91	121.13	111.82
2	A	401	NAI	C1B-N9A-C8A	2.88	133.50	127.09
2	A	401	NAI	PN-O5D-C5D	2.76	137.16	121.35
2	A	401	NAI	O3D-C3D-C4D	-2.70	103.34	111.08
2	B	401	NAI	O4D-C4D-C3D	-2.66	99.88	105.15
2	A	401	NAI	O3B-C3B-C2B	2.64	120.27	111.82
2	A	401	NAI	C2B-C3B-C4B	2.63	107.69	102.61
2	A	401	NAI	O4B-C1B-N9A	2.60	113.08	108.09
2	B	401	NAI	C1B-N9A-C8A	2.58	132.82	127.09
2	A	401	NAI	C5A-C4A-N3A	-2.55	123.20	126.72
2	A	401	NAI	C5A-C4A-N9A	2.53	108.57	105.81
2	B	401	NAI	C5A-C4A-N3A	-2.52	123.25	126.72
2	B	401	NAI	C6A-C5A-C4A	2.45	120.53	117.18
2	A	401	NAI	C6A-C5A-C4A	2.27	120.27	117.18
2	A	401	NAI	C5A-C6A-N1A	-2.24	111.81	117.51
2	A	401	NAI	N9A-C8A-N7A	2.21	117.07	113.94
2	B	401	NAI	C5A-C6A-N1A	-2.19	111.95	117.51
2	A	401	NAI	O4D-C4D-C3D	-2.13	100.92	105.15
2	A	401	NAI	O7N-C7N-C3N	-2.09	116.96	120.90
2	A	401	NAI	O3D-C3D-C2D	2.07	118.45	111.82
2	B	401	NAI	O2D-C2D-C1D	2.03	117.10	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	NAI	C1B

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAI	C5B-O5B-PA-O3
2	A	401	NAI	C4B-C5B-O5B-PA
2	B	401	NAI	C5B-O5B-PA-O1A
2	B	401	NAI	C5B-O5B-PA-O2A
2	B	401	NAI	C5B-O5B-PA-O3
2	B	401	NAI	O4B-C4B-C5B-O5B
2	B	401	NAI	C5D-O5D-PN-O3
2	B	401	NAI	C5D-O5D-PN-O1N
2	B	401	NAI	O4D-C4D-C5D-O5D
3	A	402	OXM	N1-C1-C2-O2
3	A	402	OXM	N1-C1-C2-O3
3	A	402	OXM	O1-C1-C2-O3
3	B	402	OXM	N1-C1-C2-O3
3	B	402	OXM	O1-C1-C2-O2
3	B	402	OXM	O1-C1-C2-O3
2	A	401	NAI	C3D-C4D-C5D-O5D
2	B	401	NAI	C3D-C4D-C5D-O5D
2	A	401	NAI	O4D-C4D-C5D-O5D
2	B	401	NAI	C3B-C4B-C5B-O5B
2	B	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	C2D-C1D-N1N-C2N
2	A	401	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	C5B-O5B-PA-O1A
2	A	401	NAI	O4D-C1D-N1N-C2N
2	B	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	C2D-C1D-N1N-C2N
2	A	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	O4D-C1D-N1N-C2N
2	B	401	NAI	PN-O3-PA-O2A
2	A	401	NAI	C3B-C4B-C5B-O5B
2	B	401	NAI	O4B-C1B-N9A-C8A
2	B	401	NAI	C2B-C1B-N9A-C8A

There are no ring outliers.

4 monomers are involved in 49 short contacts:

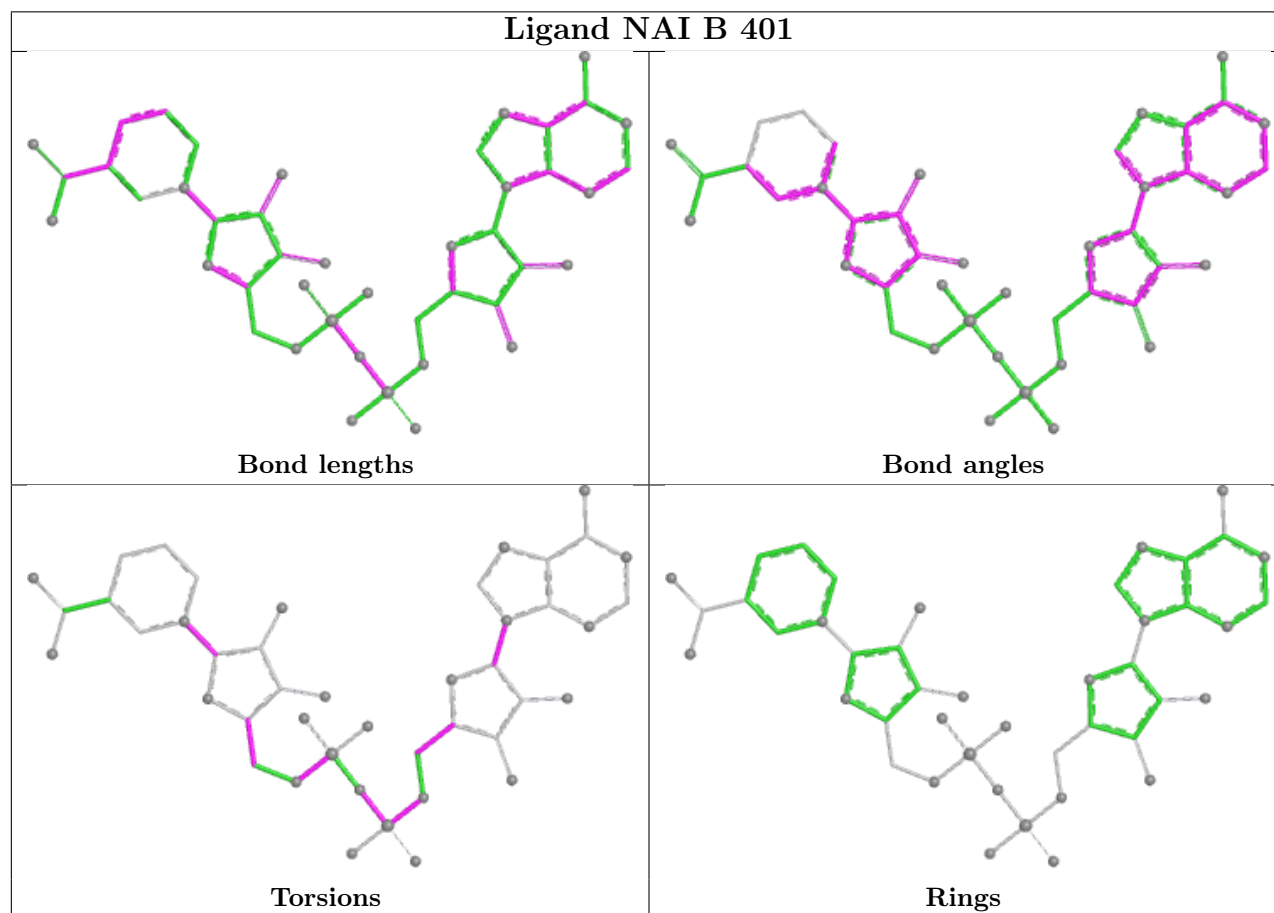
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAI	28	0

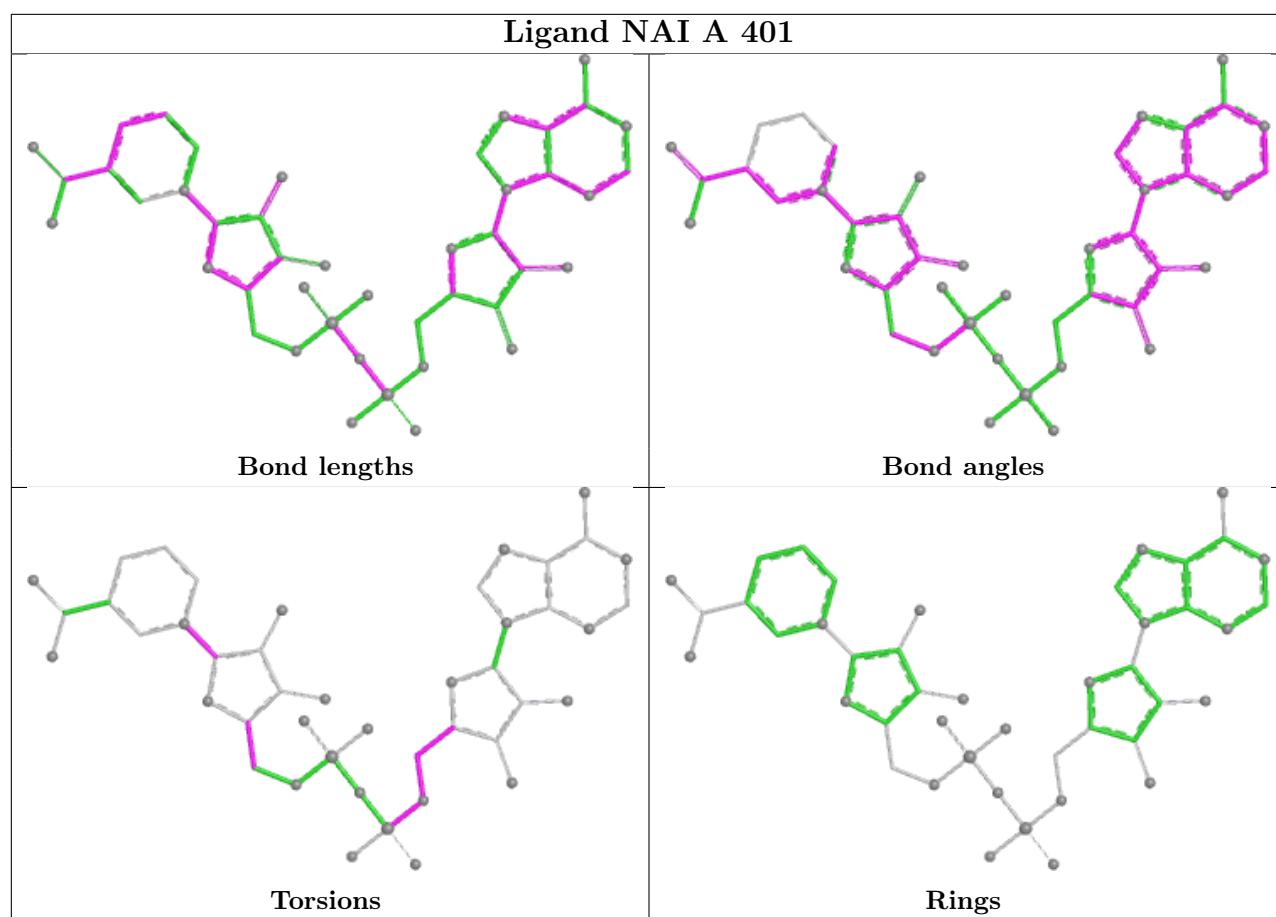
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAI	16	0
3	B	402	OXM	11	0
3	A	402	OXM	4	0

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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	337/337 (100%)	0.24	30 (8%) 15 13	2, 25, 89, 100	0
1	B	337/337 (100%)	-0.10	4 (1%) 76 75	2, 20, 70, 94	0
All	All	674/674 (100%)	0.07	34 (5%) 34 30	2, 22, 84, 100	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	TYR	4.5
1	A	31	TYR	4.3
1	A	333	ASN	4.1
1	A	8	ALA	3.6
1	B	336	LYS	3.5
1	A	41	ALA	3.3
1	A	81	VAL	3.3
1	A	62	THR	3.2
1	B	73	LYS	3.0
1	A	332	LEU	3.0
1	A	67	ALA	2.8
1	B	69	ALA	2.8
1	A	47	ALA	2.8
1	B	65	ALA	2.7
1	A	320	LEU	2.7
1	A	65	ALA	2.7
1	A	102	TYR	2.7
1	A	30	ASP	2.6
1	A	69	ALA	2.5
1	A	60	ALA	2.5
1	A	37	THR	2.5
1	A	87	ASP	2.4
1	A	83	ASN	2.4
1	A	49	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	329	PRO	2.2
1	A	26	ASP	2.2
1	A	99	VAL	2.2
1	A	57	ASP	2.2
1	A	6	ALA	2.1
1	A	40	THR	2.1
1	A	59	THR	2.1
1	A	92	LEU	2.0
1	A	27	ILE	2.0
1	A	58	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

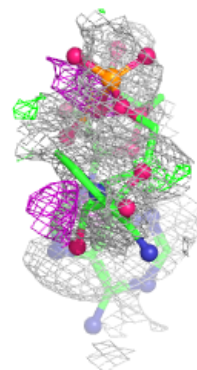
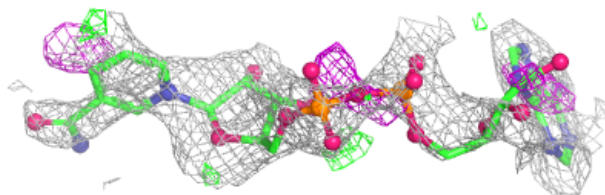
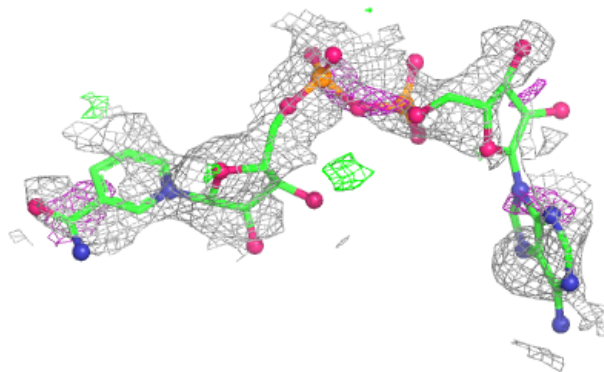
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	402	6/6	0.37	0.27	92,94,94,95	0
3	OXM	A	402	6/6	0.47	0.21	80,81,82,83	0
2	NAI	A	401	44/44	0.65	0.16	55,73,75,76	0
2	NAI	B	401	44/44	0.73	0.15	58,70,78,79	0

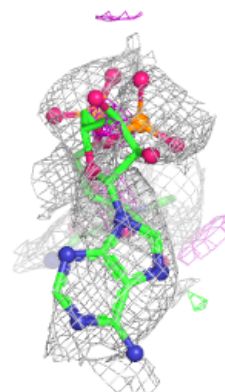
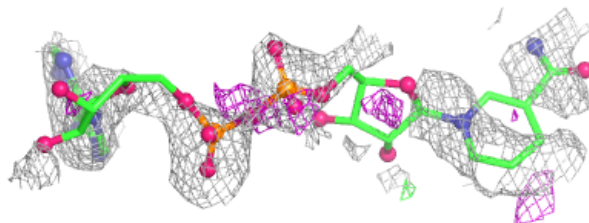
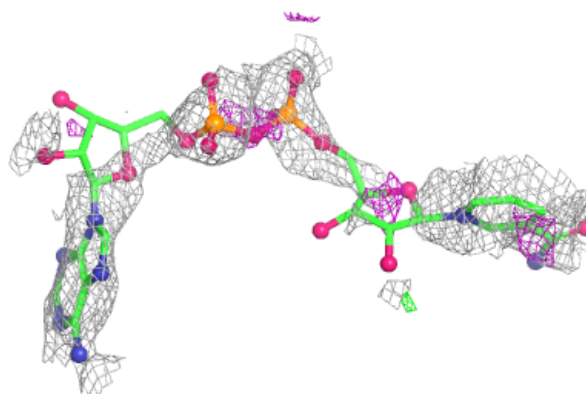
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI A 401:

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

**Electron density around NAI B 401:**

$2mF_o-DF_c$ (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.