



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:01 AM UTC

PDB ID : 1U1I / pdb_00001u1i
Title : Myo-inositol phosphate synthase mIPS from *A. fulgidus*
Authors : Stieglitz, K.A.; Yang, H.; Roberts, M.F.; Stec, B.
Deposited on : 2004-07-15
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

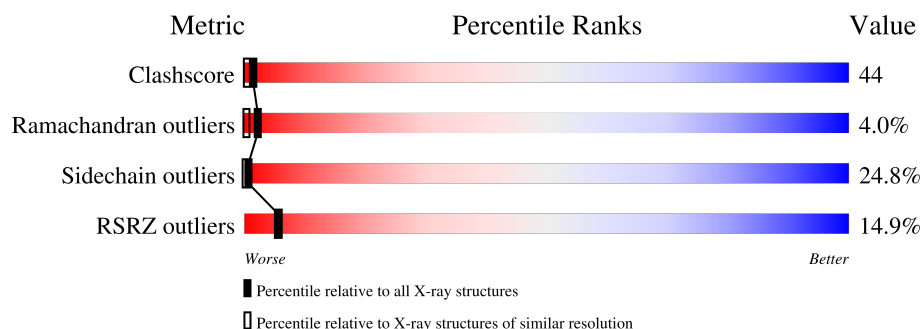
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	392	14% 30% 51% 19%
1	B	392	16% 28% 54% 17%
1	C	392	13% 30% 52% 16%
1	D	392	16% 26% 53% 19%

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	PO4	C	1195	-	-	X	-
2	PO4	D	1595	-	-	X	-

2 Entry composition [i](#)

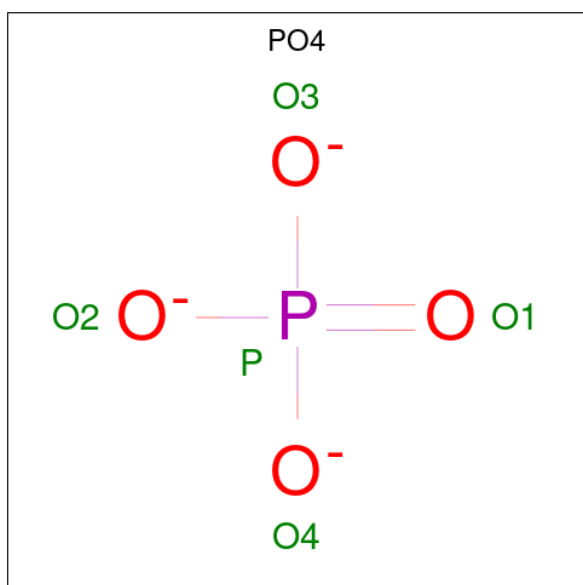
There are 5 unique types of molecules in this entry. The entry contains 13553 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 myo-inositol-1-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3084	1996	499	576	13			
1	B	392	Total	C	N	O	S	0	0	0
			3084	1996	499	576	13			
1	C	392	Total	C	N	O	S	0	0	0
			3084	1996	499	576	13			
1	D	392	Total	C	N	O	S	0	0	0
			3084	1996	499	576	13			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



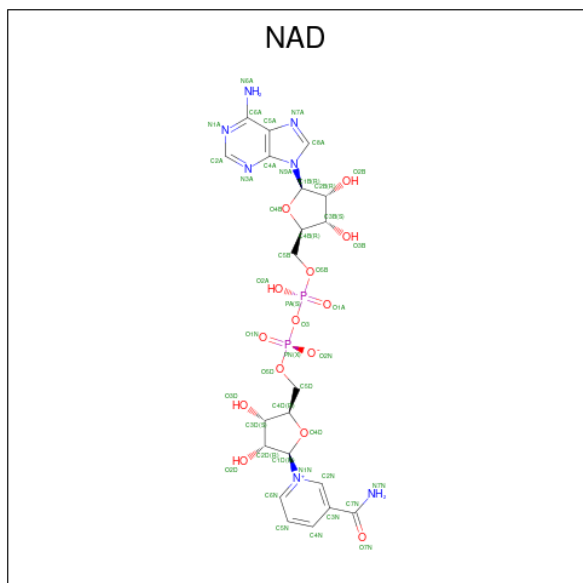
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



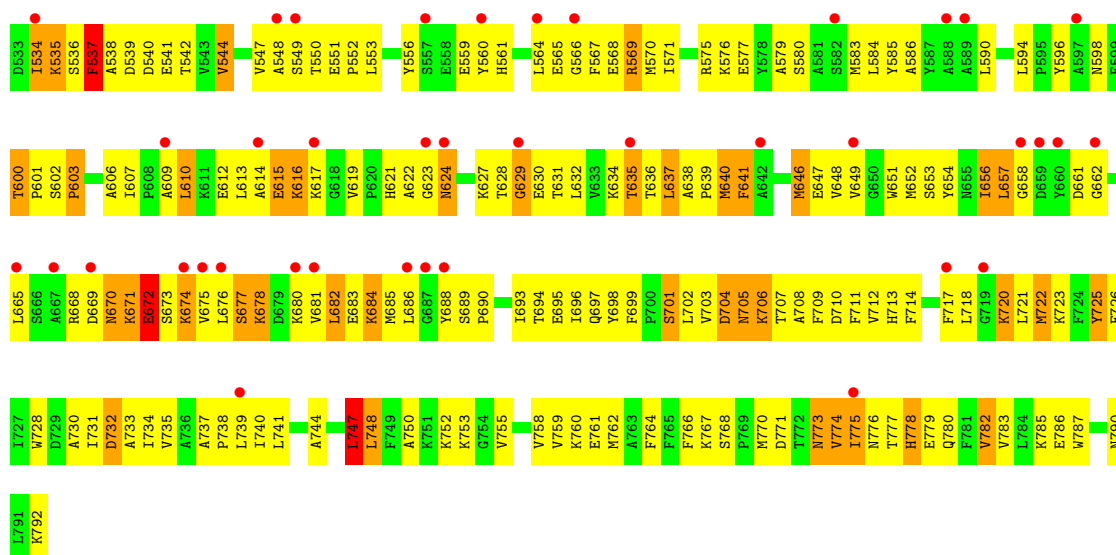
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

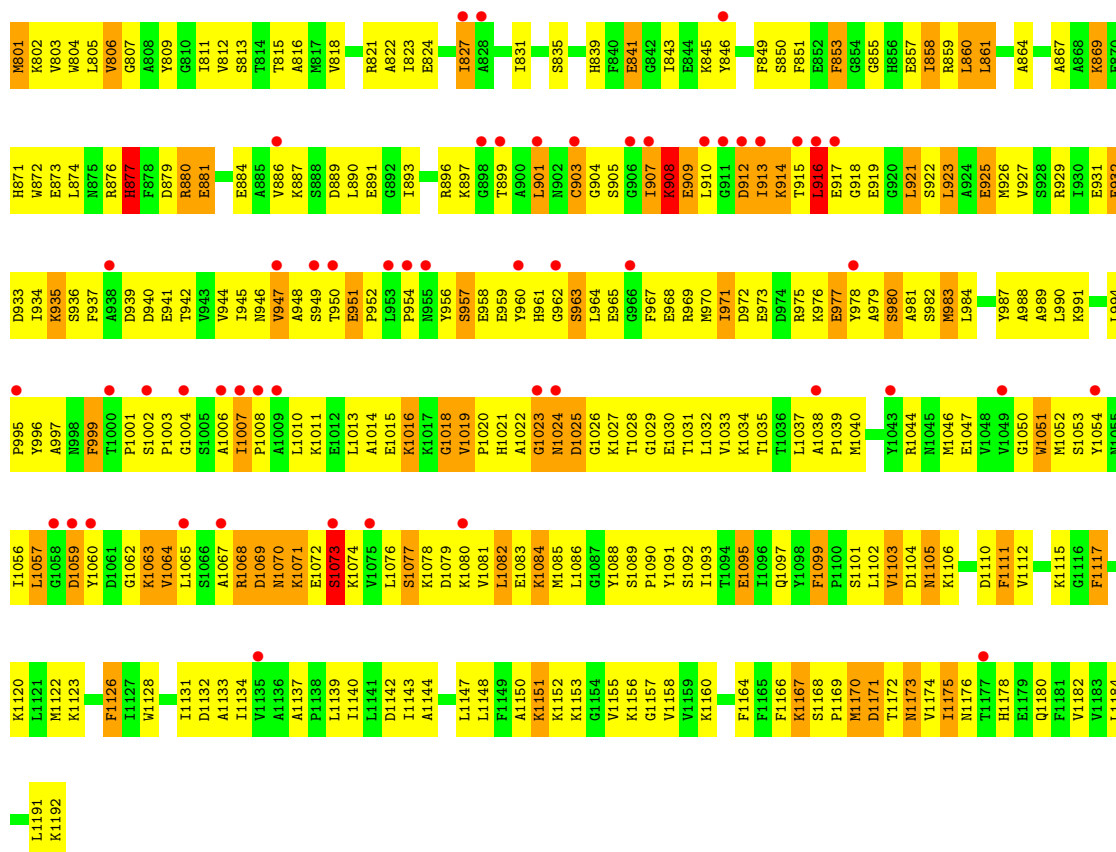
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	245	Total 245	O 245	0	0
5	B	249	Total 249	O 249	0	0
5	C	293	Total 293	O 293	0	0
5	D	232	Total 232	O 232	0	0

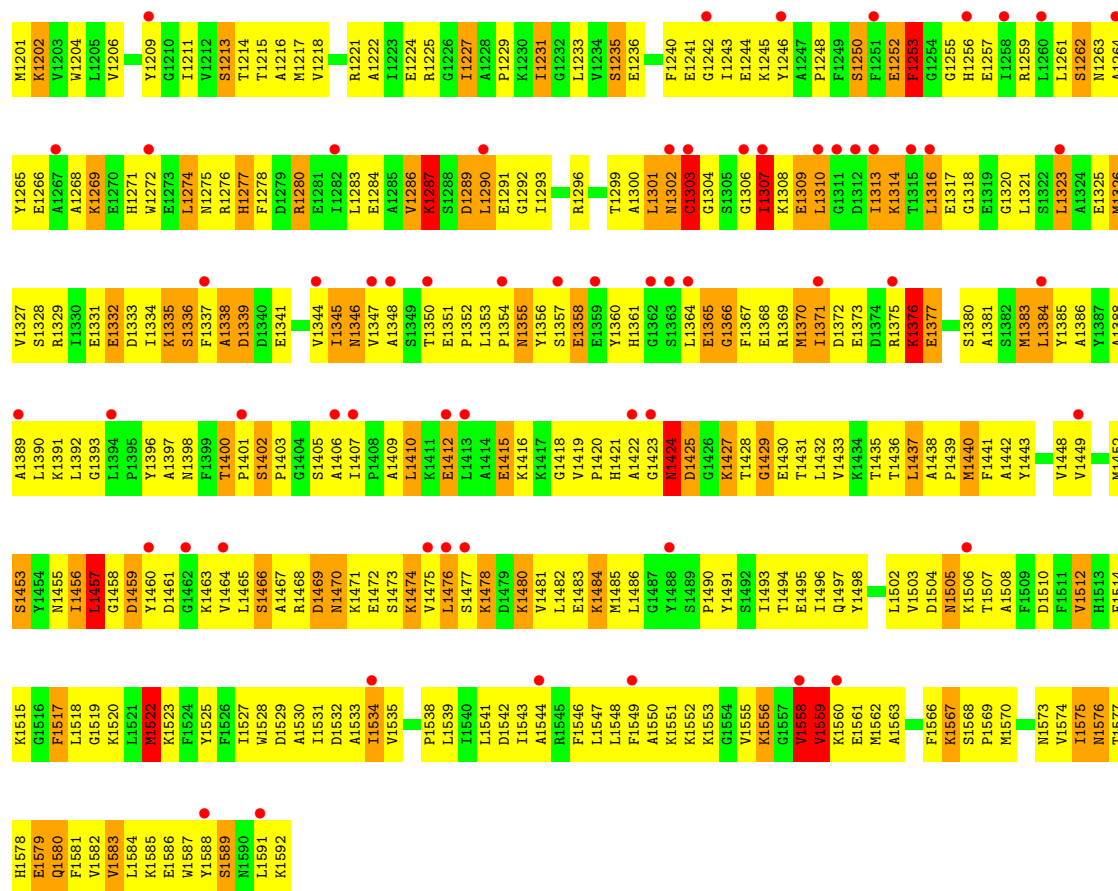


• Molecule 1: myo-inositol-1-phosphate synthase



• Molecule 1: myo-inositol-1-phosphate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.77Å 83.94Å 91.79Å 65.79° 72.43° 74.98°	Depositor
Resolution (Å)	37.60 – 1.90 37.60 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.60-1.90) 73.2 (37.60-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.89Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.211 , 0.284 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 165.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13553	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.98% 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: NAD, K, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/3155	1.31	18/4257 (0.4%)
1	B	0.37	0/3155	1.31	25/4257 (0.6%)
1	C	0.39	0/3155	1.34	35/4257 (0.8%)
1	D	0.38	0/3155	1.28	28/4257 (0.7%)
All	All	0.38	0/12620	1.31	106/17028 (0.6%)

There are no bond length outliers.

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	PHE	CA-CB-CG	10.79	124.59	113.80
1	B	699	PHE	CA-CB-CG	9.90	123.70	113.80
1	B	537	PHE	CA-CB-CG	9.69	123.49	113.80
1	C	1023	GLY	CA-C-N	9.66	139.99	121.54
1	C	1023	GLY	C-N-CA	9.66	139.99	121.54
1	D	1440	MET	CA-C-N	8.81	132.09	120.28
1	D	1440	MET	C-N-CA	8.81	132.09	120.28
1	A	222	ALA	CA-C-N	8.76	138.58	121.41
1	A	222	ALA	C-N-CA	8.76	138.58	121.41
1	C	1059	ASP	CA-CB-CG	7.86	120.46	112.60
1	C	1032	LEU	CA-C-N	7.61	130.89	120.46
1	C	1032	LEU	C-N-CA	7.61	130.89	120.46
1	B	722	MET	CA-C-N	-7.24	110.65	122.82
1	B	722	MET	C-N-CA	-7.24	110.65	122.82
1	B	704	ASP	CA-CB-CG	-7.24	105.36	112.60
1	D	1517	PHE	CA-CB-CG	7.18	120.98	113.80
1	D	1216	ALA	CA-C-N	7.17	130.48	120.29
1	D	1216	ALA	C-N-CA	7.17	130.48	120.29
1	C	801	MET	CA-C-N	-7.15	112.22	122.94
1	C	801	MET	C-N-CA	-7.15	112.22	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1128	TRP	CA-C-N	7.11	134.35	122.76
1	C	1128	TRP	C-N-CA	7.11	134.35	122.76
1	C	1144	ALA	CA-C-N	7.06	130.31	120.29
1	C	1144	ALA	C-N-CA	7.06	130.31	120.29
1	C	1019	VAL	O-C-N	7.03	127.48	120.59
1	B	747	LEU	CA-C-N	6.92	129.85	120.44
1	B	747	LEU	C-N-CA	6.92	129.85	120.44
1	C	1126	PHE	CA-CB-CG	6.74	120.54	113.80
1	B	443	ILE	CA-C-N	6.63	131.30	120.63
1	B	443	ILE	C-N-CA	6.63	131.30	120.63
1	C	1018	GLY	CA-C-N	-6.63	117.09	122.85
1	C	1018	GLY	C-N-CA	-6.63	117.09	122.85
1	D	1427	LYS	CA-C-N	6.56	130.83	121.71
1	D	1427	LYS	C-N-CA	6.56	130.83	121.71
1	C	803	VAL	CA-C-N	-6.52	113.85	123.11
1	C	803	VAL	C-N-CA	-6.52	113.85	123.11
1	B	672	GLU	CA-C-N	6.49	128.88	120.44
1	B	672	GLU	C-N-CA	6.49	128.88	120.44
1	C	853	PHE	CA-C-N	6.49	129.77	120.56
1	C	853	PHE	C-N-CA	6.49	129.77	120.56
1	D	1253	PHE	CA-C-N	6.32	130.57	121.03
1	D	1253	PHE	C-N-CA	6.32	130.57	121.03
1	B	705	ASN	CA-CB-CG	6.23	118.83	112.60
1	B	646	MET	CA-C-N	-6.22	114.14	122.72
1	B	646	MET	C-N-CA	-6.22	114.14	122.72
1	C	1051	TRP	CA-C-N	-6.22	114.42	123.00
1	C	1051	TRP	C-N-CA	-6.22	114.42	123.00
1	A	363	ALA	CA-C-N	6.15	130.53	120.63
1	A	363	ALA	C-N-CA	6.15	130.53	120.63
1	B	480	ARG	CA-C-N	6.08	129.04	120.28
1	B	480	ARG	C-N-CA	6.08	129.04	120.28
1	D	1505	ASN	CA-CB-CG	6.01	118.61	112.60
1	D	1522	MET	CA-C-N	-5.96	113.31	122.62
1	D	1522	MET	C-N-CA	-5.96	113.31	122.62
1	C	1173	ASN	CA-C-N	5.94	131.19	123.11
1	C	1173	ASN	C-N-CA	5.94	131.19	123.11
1	D	1523	LYS	CA-C-N	-5.82	111.76	121.89
1	D	1523	LYS	C-N-CA	-5.82	111.76	121.89
1	D	1441	PHE	CA-C-N	5.82	128.35	120.44
1	D	1441	PHE	C-N-CA	5.82	128.35	120.44
1	A	77	HIS	CA-CB-CG	5.80	119.60	113.80
1	A	244	ARG	CA-C-N	5.79	130.59	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ARG	C-N-CA	5.79	130.59	122.08
1	A	87	LYS	CA-C-N	5.73	127.96	120.28
1	A	87	LYS	C-N-CA	5.73	127.96	120.28
1	B	722	MET	O-C-N	-5.72	116.52	123.10
1	B	671	LYS	CA-C-N	5.69	128.70	120.79
1	B	671	LYS	C-N-CA	5.69	128.70	120.79
1	D	1576	ASN	CA-CB-CG	5.65	118.25	112.60
1	B	732	ASP	CA-CB-CG	-5.64	106.95	112.60
1	D	1341	GLU	CA-C-N	-5.64	115.22	123.00
1	D	1341	GLU	C-N-CA	-5.64	115.22	123.00
1	D	1523	LYS	CA-C-O	5.62	127.69	121.11
1	C	1184	LEU	CA-C-N	5.61	127.74	120.44
1	C	1184	LEU	C-N-CA	5.61	127.74	120.44
1	D	1476	LEU	CA-C-N	5.56	130.00	120.72
1	D	1476	LEU	C-N-CA	5.56	130.00	120.72
1	A	269	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	432	GLY	CA-C-N	-5.48	115.49	122.77
1	B	432	GLY	C-N-CA	-5.48	115.49	122.77
1	C	877	HIS	CA-CB-CG	5.44	119.24	113.80
1	D	1286	VAL	N-CA-C	-5.43	107.45	112.83
1	A	223	GLY	CA-C-N	5.40	131.85	121.54
1	A	223	GLY	C-N-CA	5.40	131.85	121.54
1	D	1512	VAL	CB-CA-C	-5.38	103.71	111.19
1	B	670	ASN	CA-C-N	5.38	128.48	120.31
1	B	670	ASN	C-N-CA	5.38	128.48	120.31
1	A	269	ASP	CA-C-N	5.37	127.94	120.63
1	A	269	ASP	C-N-CA	5.37	127.94	120.63
1	D	1301	LEU	CA-C-N	5.27	131.61	121.54
1	D	1301	LEU	C-N-CA	5.27	131.61	121.54
1	D	1498	TYR	CA-C-N	5.25	128.87	122.42
1	D	1498	TYR	C-N-CA	5.25	128.87	122.42
1	C	1032	LEU	O-C-N	5.21	127.45	122.03
1	C	983	MET	CA-C-N	5.20	127.68	120.29
1	C	983	MET	C-N-CA	5.20	127.68	120.29
1	A	314	PHE	CA-CB-CG	5.19	118.99	113.80
1	C	839	HIS	CA-C-N	-5.13	114.51	122.67
1	C	839	HIS	C-N-CA	-5.13	114.51	122.67
1	C	1099	PHE	O-C-N	5.11	127.19	121.32
1	B	477	HIS	CA-CB-CG	5.09	118.89	113.80
1	A	385	LYS	CA-C-N	5.06	127.32	120.44
1	A	385	LYS	C-N-CA	5.06	127.32	120.44
1	C	999	PHE	CA-CB-CG	5.03	118.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1111	PHE	CA-C-N	-5.03	116.42	123.10
1	C	1111	PHE	C-N-CA	-5.03	116.42	123.10

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	3084	0	3084	273	0
1	B	3084	0	3081	283	0
1	C	3084	0	3081	275	0
1	D	3084	0	3081	310	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	2	0
2	D	5	0	0	2	0
3	A	44	0	26	6	0
3	B	44	0	26	5	0
3	C	44	0	26	8	0
3	D	44	0	25	9	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	245	0	0	17	0
5	B	249	0	0	16	0
5	C	293	0	0	5	0
5	D	232	0	0	8	0
All	All	13553	0	12430	1094	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 44.

All (1094) 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:C:916:LEU:HD11	1:C:926:MET:CG	1.46	1.45
1:C:916:LEU:HD12	1:C:926:MET:SD	1.52	1.45
1:C:916:LEU:CD1	1:C:926:MET:HG2	1.51	1.38
1:C:916:LEU:CD1	1:C:926:MET:CG	2.03	1.36
1:C:916:LEU:CD1	1:C:926:MET:SD	2.19	1.28
1:A:233:VAL:HG22	1:B:640:MET:HE1	1.38	1.04
1:C:916:LEU:HD11	1:C:926:MET:HG2	1.04	1.01
1:D:1398:ASN:HD22	1:D:1424:ASN:HA	1.23	1.01
1:B:411:ILE:HD12	1:B:471:HIS:HB3	1.42	1.00
1:D:1280:ARG:HD2	1:D:1283:LEU:HD23	1.46	0.98
1:C:916:LEU:HD11	1:C:926:MET:CB	1.95	0.96
1:D:1351:GLU:HG2	1:D:1402:SER:HB2	1.46	0.96
1:C:1006:ALA:HA	1:C:1170:MET:HE3	1.48	0.96
1:A:170:MET:HG3	1:A:175:ARG:HB2	1.45	0.96
1:D:1428:THR:HG21	3:D:1596:NAD:H71N	1.32	0.93
1:C:1084:LYS:HB3	1:C:1173:ASN:HD21	1.34	0.93
1:B:523:LEU:HD13	1:B:576:LYS:HG2	1.51	0.92
1:D:1476:LEU:HD22	1:D:1480:LYS:HZ2	1.32	0.92
1:B:776:ASN:HB3	1:B:779:GLU:HB2	1.51	0.91
1:A:58:ILE:HD12	1:A:110:LEU:HD11	1.51	0.91
1:C:859:ARG:HG3	1:C:910:LEU:HD11	1.51	0.91
1:C:1040:MET:HE1	1:D:1433:VAL:HA	1.51	0.91
1:D:1217:MET:HE1	1:D:1293:ILE:HG21	1.53	0.90
1:A:11:ILE:HG13	1:A:71:HIS:HB3	1.52	0.90
1:D:1316:LEU:HD21	1:D:1326:MET:HG2	1.55	0.89
1:A:97:LYS:HE3	1:A:113:ILE:HD11	1.53	0.89
1:C:1131:ILE:HB	1:D:1520:LYS:HE2	1.53	0.89
1:C:1134:ILE:HG12	1:D:1520:LYS:HD3	1.55	0.86
1:A:257:LEU:HG	1:A:306:LYS:HG3	1.56	0.85
1:A:90:LEU:HA	1:A:93:ILE:HD12	1.58	0.84
1:C:916:LEU:HD12	1:C:926:MET:CG	1.89	0.84
1:C:1065:LEU:HD22	1:C:1071:LYS:HA	1.60	0.83
1:A:173:GLU:HB3	1:A:175:ARG:HD3	1.60	0.83
1:B:417:MET:HE2	1:B:453:PHE:HB3	1.59	0.83
1:C:801:MET:HE3	1:C:1148:LEU:HD22	1.61	0.82
1:D:1364:LEU:HD11	1:D:1412:GLU:HB3	1.62	0.82
1:B:695:GLU:HG2	1:B:697:GLN:HE21	1.45	0.81
1:B:510:LEU:HA	1:B:513:ILE:HD12	1.63	0.81
1:A:97:LYS:HG2	1:A:115:THR:HB	1.62	0.81
1:B:606:ALA:HB2	1:B:624:ASN:HD21	1.45	0.81
1:D:1567:LYS:HE2	2:D:1595:PO4:O4	1.81	0.81
1:C:923:LEU:HD23	1:C:971:ILE:HA	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1474:LYS:HE2	1:D:1567:LYS:HZ1	1.45	0.80
1:B:523:LEU:HD21	1:B:579:ALA:HB2	1.62	0.80
1:C:877:HIS:HB2	1:C:1134:ILE:HD11	1.64	0.79
1:B:576:LYS:HB3	5:B:2404:HOH:O	1.83	0.79
1:B:553:LEU:HD13	1:B:672:GLU:OE2	1.83	0.79
1:B:680:LYS:HZ2	1:B:684:LYS:HB2	1.48	0.79
1:D:1354:PRO:HB3	1:D:1403:PRO:HG3	1.64	0.79
1:A:61:LEU:HD12	1:A:67:ALA:HB2	1.65	0.78
1:C:909:GLU:O	1:C:910:LEU:HD13	1.83	0.78
1:B:522:SER:O	1:B:526:MET:HG3	1.83	0.78
1:B:598:ASN:OD1	1:B:600:THR:HG23	1.84	0.78
1:B:661:ASP:O	1:B:665:LEU:HG	1.84	0.78
1:C:1040:MET:HE2	1:D:1432:LEU:HG	1.65	0.78
1:A:272:GLU:O	1:A:276:LEU:HG	1.84	0.78
1:D:1284:GLU:O	1:D:1287:LYS:HB2	1.83	0.78
1:B:678:LYS:HB3	1:B:694:THR:HG21	1.66	0.78
1:C:1028:THR:OG1	3:C:1196:NAD:H4N	1.84	0.78
1:A:114:LYS:HG2	1:A:119:GLU:HA	1.66	0.77
1:B:782:VAL:HA	1:B:785:LYS:HD3	1.64	0.77
1:D:1532:ASP:HB3	3:D:1596:NAD:H72N	1.48	0.77
1:C:904:GLY:O	1:C:907:ILE:HG13	1.84	0.77
1:C:1069:ASP:O	1:C:1072:GLU:HB3	1.85	0.77
1:C:1031:THR:O	1:C:1035:THR:HG23	1.85	0.77
1:D:1217:MET:HE3	1:D:1253:PHE:HB2	1.66	0.76
1:D:1421:HIS:O	1:D:1558:VAL:HA	1.85	0.76
1:B:409:TYR:HE2	1:B:461:LEU:H	1.34	0.76
1:D:1214:THR:O	1:D:1218:VAL:HG23	1.85	0.76
1:A:131:GLU:O	1:A:135:LYS:HB2	1.86	0.75
1:C:980:SER:HB3	1:C:983:MET:HE3	1.67	0.75
1:C:990:LEU:HD22	1:C:1014:ALA:HB2	1.67	0.75
1:D:1277:HIS:O	1:D:1534:ILE:HD11	1.86	0.75
1:C:1077:SER:O	1:C:1081:VAL:HG23	1.87	0.75
1:B:637:LEU:O	1:B:640:MET:HB3	1.86	0.75
1:A:11:ILE:HD13	1:A:333:ALA:HB2	1.68	0.75
1:B:460:LEU:HD21	1:B:495:ALA:O	1.87	0.75
1:C:1014:ALA:HB1	1:C:1019:VAL:O	1.85	0.75
1:A:367:LYS:HE2	2:A:395:PO4:O4	1.87	0.74
1:D:1424:ASN:O	1:D:1566:PHE:HB3	1.88	0.74
1:A:376:ASN:HB3	1:A:379:GLU:HB2	1.67	0.74
1:A:252:MET:HE3	1:A:254:TYR:HB2	1.70	0.74
1:B:490:LEU:HA	1:B:493:ILE:HG13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:VAL:HG22	3:B:796:NAD:H51N	1.68	0.74
1:D:1299:THR:HG21	1:D:1384:LEU:HD12	1.69	0.74
1:D:1468:ARG:HH22	1:D:1472:GLU:HG3	1.53	0.74
1:A:154:PRO:HG3	1:A:203:PRO:HG3	1.69	0.74
1:A:260:TYR:HA	1:A:263:LYS:HG3	1.69	0.74
1:D:1448:VAL:O	1:D:1490:PRO:HB3	1.85	0.74
1:D:1253:PHE:O	1:D:1293:ILE:HD12	1.88	0.74
1:D:1515:LYS:HE3	1:D:1519:GLY:HA2	1.70	0.74
1:A:254:TYR:OH	1:A:297:GLN:HG3	1.88	0.74
1:B:613:LEU:O	1:B:617:LYS:HB2	1.88	0.73
1:C:1160:LYS:HG2	1:C:1171:ASP:HB2	1.69	0.73
1:A:269:ASP:HB2	1:A:270:ASN:OD1	1.88	0.73
1:B:671:LYS:HE2	1:B:675:VAL:HG21	1.69	0.73
1:C:922:SER:OG	1:C:925:GLU:HG3	1.88	0.73
1:B:430:LYS:HE3	5:B:2422:HOH:O	1.87	0.73
1:B:522:SER:OG	1:B:525:GLU:HB2	1.89	0.73
1:D:1327:VAL:HG21	1:D:1371:ILE:HD11	1.71	0.73
1:D:1398:ASN:ND2	1:D:1424:ASN:HA	2.03	0.72
1:B:564:LEU:HB3	5:B:1792:HOH:O	1.89	0.72
1:C:884:GLU:O	1:C:887:LYS:HB3	1.89	0.72
1:C:1026:GLY:O	3:C:1196:NAD:H5N	1.89	0.72
1:D:1259:ARG:HG2	1:D:1310:LEU:HG	1.71	0.72
1:D:1364:LEU:HD12	1:D:1364:LEU:H	1.53	0.72
1:A:102:ASN:HB3	5:A:1976:HOH:O	1.88	0.72
1:A:161:HIS:HE1	1:A:170:MET:HE1	1.53	0.72
1:B:559:GLU:HB2	1:B:569:ARG:HH12	1.53	0.72
1:A:96:ARG:HD3	1:A:133:ASP:HB3	1.71	0.72
1:D:1428:THR:HG21	3:D:1596:NAD:N7N	2.05	0.72
1:C:1151:LYS:HE2	5:C:2191:HOH:O	1.89	0.72
1:C:922:SER:O	1:C:926:MET:HG3	1.90	0.72
1:D:1393:GLY:HA2	1:D:1419:VAL:HG21	1.72	0.72
1:C:921:LEU:HD21	1:C:929:ARG:NH1	2.04	0.71
1:D:1331:GLU:HG3	1:D:1388:ALA:HB1	1.70	0.71
1:D:1242:GLY:O	1:D:1245:LYS:HG2	1.89	0.71
1:D:1357:SER:H	1:D:1361:HIS:HD2	1.37	0.71
1:C:923:LEU:O	1:C:927:VAL:HG23	1.90	0.71
1:C:919:GLU:HB2	1:C:921:LEU:HD13	1.73	0.71
1:C:964:LEU:HD21	1:C:1013:LEU:HD13	1.70	0.71
1:C:1117:PHE:HA	1:D:1231:ILE:O	1.90	0.71
1:A:240:MET:HB2	1:B:636:THR:HG21	1.72	0.71
1:B:583:MET:HE2	1:B:607:ILE:HD13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1242:GLY:O	1:D:1245:LYS:HE2	1.90	0.71
1:D:1364:LEU:O	1:D:1368:GLU:HB2	1.91	0.71
1:C:1037:LEU:O	1:C:1040:MET:HB3	1.91	0.70
1:C:1153:LYS:HB3	1:C:1191:LEU:HD22	1.74	0.70
1:C:1178:HIS:O	1:C:1182:VAL:HG23	1.92	0.70
1:A:318:LEU:HD21	1:B:419:GLY:HA2	1.73	0.70
1:B:411:ILE:HG12	1:B:733:ALA:HB2	1.74	0.70
1:C:811:ILE:HD12	1:C:871:HIS:HB3	1.72	0.70
1:A:249:VAL:HG23	1:A:313:HIS:O	1.92	0.70
1:B:774:VAL:HG13	1:B:779:GLU:OE2	1.91	0.70
1:D:1397:ALA:HB2	1:D:1547:LEU:HD11	1.74	0.69
1:B:641:PHE:HB3	1:B:646:MET:HB2	1.74	0.69
1:D:1587:TRP:O	1:D:1591:LEU:HG	1.91	0.69
1:A:6:VAL:HG12	1:A:148:ALA:HB2	1.75	0.69
1:B:776:ASN:O	1:B:780:GLN:HG3	1.92	0.69
1:C:821:ARG:HD2	1:C:889:ASP:OD1	1.92	0.69
1:A:127:VAL:HG21	1:A:171:ILE:HD12	1.74	0.69
1:B:677:SER:HB2	1:B:767:LYS:HD2	1.75	0.69
1:B:497:LYS:H	1:B:497:LYS:HD2	1.56	0.69
1:A:127:VAL:HG22	1:A:184:LEU:HD22	1.74	0.69
1:C:1067:ALA:O	1:C:1071:LYS:HD2	1.92	0.68
1:A:201:PRO:HB3	1:A:225:ASP:OD2	1.93	0.68
1:A:213:LEU:O	1:A:217:LYS:HD3	1.93	0.68
1:C:899:THR:HB	1:C:916:LEU:HD23	1.75	0.68
1:C:1117:PHE:HB2	1:D:1538:PRO:HG3	1.76	0.68
1:B:720:LYS:HE2	1:B:721:LEU:O	1.94	0.68
1:B:708:ALA:HB3	1:B:728:TRP:HB3	1.75	0.68
1:A:223:GLY:O	1:A:370:MET:HG3	1.94	0.67
1:B:484:GLU:O	1:B:487:LYS:HB3	1.94	0.67
1:B:420:ALA:O	1:B:424:GLU:HG3	1.94	0.67
1:B:544:VAL:O	1:B:596:TYR:HA	1.94	0.67
1:D:1202:LYS:HD3	1:D:1339:ASP:OD2	1.95	0.67
1:B:480:ARG:HB2	5:B:1611:HOH:O	1.93	0.67
1:D:1303:CYS:HB3	1:D:1352:PRO:HD2	1.77	0.67
1:D:1467:ALA:O	1:D:1471:LYS:HB2	1.94	0.67
1:B:668:ARG:HA	1:B:671:LYS:HB3	1.77	0.67
1:A:205:SER:HA	1:A:210:LEU:HD12	1.77	0.67
1:C:916:LEU:CG	1:C:926:MET:SD	2.82	0.66
1:D:1429:GLY:O	1:D:1433:VAL:HG23	1.96	0.66
1:B:421:ARG:O	1:B:425:ARG:HG3	1.95	0.66
1:C:915:THR:O	1:C:919:GLU:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:999:PHE:O	1:C:1025:ASP:HA	1.94	0.66
1:C:1020:PRO:HA	1:C:1157:GLY:O	1.96	0.66
1:C:1115:LYS:HG3	1:C:1120:LYS:O	1.95	0.66
1:D:1381:ALA:O	1:D:1384:LEU:HB2	1.95	0.66
1:A:22:ALA:O	1:A:27:ILE:HG13	1.95	0.66
1:B:469:LYS:O	1:B:473:GLU:HG2	1.95	0.66
1:B:501:LEU:HD23	1:B:517:GLU:OE1	1.96	0.66
1:D:1329:ARG:HA	1:D:1332:GLU:HB2	1.78	0.66
1:B:552:PRO:HD3	1:B:670:ASN:OD1	1.96	0.66
1:C:1067:ALA:O	1:C:1071:LYS:HB3	1.96	0.65
1:D:1302:ASN:ND2	1:D:1377:GLU:HA	2.11	0.65
1:B:424:GLU:OE1	1:B:450:SER:HA	1.96	0.65
1:A:225:ASP:OD1	1:A:367:LYS:HE3	1.96	0.65
1:B:550:THR:HG23	1:B:601:PRO:HD2	1.78	0.65
1:B:556:TYR:HA	1:B:561:HIS:ND1	2.11	0.65
1:C:824:GLU:OE2	1:C:850:SER:HA	1.96	0.65
1:B:761:GLU:HG2	1:B:787:TRP:HB2	1.77	0.65
1:C:1024:ASN:HB2	1:C:1168:SER:O	1.95	0.65
1:B:559:GLU:HB2	1:B:569:ARG:NH1	2.11	0.65
1:A:4:TRP:HH2	1:A:96:ARG:HD2	1.61	0.65
1:C:960:TYR:HB3	1:C:970:MET:HB2	1.79	0.65
1:C:1176:ASN:O	1:C:1180:GLN:HG3	1.97	0.65
1:A:104:GLY:HA3	1:A:152:PRO:HG3	1.77	0.65
1:C:1016:LYS:HG3	1:C:1016:LYS:O	1.96	0.65
1:B:549:SER:HB2	3:B:796:NAD:H8A	1.79	0.65
1:B:462:SER:O	1:B:494:VAL:HG22	1.97	0.64
1:D:1213:SER:O	1:D:1217:MET:HG3	1.98	0.64
1:D:1435:THR:HA	1:D:1485:MET:HE1	1.80	0.64
1:A:56:HIS:HB2	5:A:2000:HOH:O	1.97	0.64
1:D:1400:THR:OG1	1:D:1402:SER:HB3	1.97	0.64
1:C:1064:VAL:HG13	1:C:1070:ASN:HD22	1.61	0.64
1:A:372:THR:HG23	1:A:374:VAL:H	1.63	0.64
1:D:1365:GLU:HA	5:D:1818:HOH:O	1.97	0.64
1:D:1272:TRP:CH2	1:D:1280:ARG:HB2	2.33	0.64
1:A:190:LEU:HD13	1:A:214:ALA:HB2	1.79	0.64
1:D:1265:TYR:N	1:D:1290:LEU:HB3	2.13	0.64
1:D:1475:VAL:O	1:D:1478:LYS:HG3	1.98	0.64
1:A:122:SER:OG	1:A:125:GLU:HG3	1.97	0.64
1:D:1229:PRO:HB2	1:D:1231:ILE:HG12	1.80	0.63
1:D:1390:LEU:HD12	1:D:1410:LEU:HD13	1.81	0.63
1:A:250:GLY:HA2	1:A:291:TYR:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:GLU:HG3	1:B:510:LEU:HD13	1.80	0.63
1:B:515:THR:HG23	1:B:519:GLU:OE1	1.98	0.63
1:D:1368:GLU:HB3	5:D:1818:HOH:O	1.98	0.63
1:B:438:PRO:O	1:B:441:GLU:HB2	1.98	0.63
1:A:197:ALA:HB2	1:A:347:LEU:HD11	1.80	0.63
1:A:232:LEU:HD13	1:B:640:MET:SD	2.38	0.63
1:D:1303:CYS:SG	1:D:1352:PRO:HG2	2.39	0.63
1:A:148:ALA:O	3:A:396:NAD:H4D	1.97	0.63
1:A:356:LYS:HG2	5:A:1863:HOH:O	1.98	0.63
1:B:519:GLU:HG2	5:B:2276:HOH:O	1.99	0.63
1:B:409:TYR:HB2	1:B:457:GLU:OE2	1.98	0.63
1:A:228:THR:HB	1:A:335:VAL:HG23	1.81	0.63
1:A:158:GLU:HG3	1:A:158:GLU:O	1.98	0.63
1:B:426:GLY:HA2	5:B:2115:HOH:O	1.98	0.63
1:C:1106:LYS:HB3	1:C:1132:ASP:OD1	1.99	0.63
1:A:230:GLU:OE1	1:A:308:ALA:HB1	1.99	0.63
1:B:560:TYR:CD2	1:B:570:MET:HB2	2.34	0.62
1:C:1025:ASP:O	1:C:1166:PHE:HA	1.99	0.62
1:D:1272:TRP:CZ3	1:D:1280:ARG:HD3	2.35	0.62
1:A:220:PRO:HB3	1:A:355:VAL:HG12	1.82	0.62
1:A:65:TYR:CE1	1:A:87:LYS:HB2	2.35	0.62
1:D:1456:ILE:HD12	1:D:1502:LEU:HD11	1.81	0.62
1:A:378:HIS:ND1	1:B:778:HIS:HB2	2.15	0.61
1:B:741:LEU:O	1:B:744:ALA:HB3	1.99	0.61
1:D:1476:LEU:HD22	1:D:1480:LYS:NZ	2.11	0.61
1:B:669:ASP:HB2	5:B:1830:HOH:O	2.01	0.61
1:D:1369:ARG:O	1:D:1373:GLU:HG3	2.01	0.61
1:A:161:HIS:O	1:A:208:PRO:HD2	2.01	0.61
1:A:235:THR:HA	1:A:285:MET:SD	2.40	0.61
1:B:472:TRP:CH2	1:B:480:ARG:HG3	2.36	0.61
1:C:956:TYR:OH	1:C:1008:PRO:HG2	2.00	0.61
1:D:1581:PHE:CE2	1:D:1585:LYS:HD2	2.36	0.61
1:B:487:LYS:HD3	5:B:2073:HOH:O	2.00	0.61
1:B:517:GLU:HB2	1:B:526:MET:SD	2.40	0.61
1:D:1383:MET:HE1	5:D:2579:HOH:O	1.99	0.61
1:D:1448:VAL:HG12	1:D:1490:PRO:HB3	1.83	0.61
1:D:1506:LYS:HD2	1:D:1532:ASP:OD2	2.00	0.61
1:A:311:PHE:CE2	1:A:323:LYS:HB3	2.35	0.60
1:B:586:ALA:O	1:B:590:LEU:HG	2.01	0.60
1:D:1323:LEU:HD22	1:D:1376:LYS:HG3	1.82	0.60
1:C:804:TRP:CE2	1:C:855:GLY:HA2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1064:VAL:HG13	1:C:1070:ASN:ND2	2.16	0.60
1:A:257:LEU:HB3	1:A:306:LYS:HA	1.83	0.60
1:B:652:MET:HE3	1:B:709:PHE:O	2.01	0.60
1:C:809:TYR:CD2	1:C:857:GLU:HG2	2.36	0.60
1:D:1357:SER:H	1:D:1361:HIS:CD2	2.19	0.60
1:C:948:ALA:O	3:C:1196:NAD:H4D	2.02	0.60
1:C:964:LEU:O	1:C:968:GLU:HG3	2.02	0.60
1:A:58:ILE:O	1:A:110:LEU:HD22	2.02	0.60
1:A:97:LYS:O	1:A:116:LEU:HD23	2.02	0.60
1:A:152:PRO:HB3	1:A:269:ASP:HB3	1.81	0.60
1:D:1552:LYS:O	1:D:1553:LYS:HD3	2.01	0.60
1:D:1532:ASP:HB3	3:D:1596:NAD:N7N	2.17	0.60
1:A:149:SER:H	3:A:396:NAD:C8A	2.15	0.60
1:B:602:SER:OG	1:B:603:PRO:HD2	2.02	0.59
1:A:374:VAL:HG13	1:A:379:GLU:HB3	1.83	0.59
1:C:802:LYS:HD2	1:C:939:ASP:OD1	2.03	0.59
1:C:958:GLU:HG3	5:C:1985:HOH:O	2.02	0.59
1:D:1368:GLU:O	1:D:1371:ILE:HG22	2.02	0.59
1:B:758:VAL:HG21	1:B:771:ASP:OD2	2.01	0.59
1:C:970:MET:HE3	1:C:979:ALA:HB2	1.84	0.59
1:B:409:TYR:CD2	1:B:457:GLU:HG2	2.37	0.59
1:B:634:LYS:HD3	1:B:682:LEU:HD13	1.84	0.59
1:C:896:ARG:HD2	1:C:933:ASP:OD2	2.03	0.59
1:B:758:VAL:HG11	1:B:770:MET:HB2	1.85	0.59
1:D:1459:ASP:O	1:D:1463:LYS:HG3	2.02	0.59
1:A:130:ILE:O	1:A:134:ILE:HG22	2.03	0.59
1:B:470:GLU:O	1:B:473:GLU:HB2	2.03	0.59
1:B:514:LYS:HD2	1:B:518:GLY:H	1.67	0.59
1:B:570:MET:HE3	1:B:579:ALA:HB2	1.82	0.59
1:A:256:ILE:HD12	1:A:302:LEU:HD11	1.84	0.59
1:D:1217:MET:HB3	1:D:1221:ARG:HH12	1.67	0.59
1:D:1329:ARG:O	1:D:1332:GLU:HB2	2.03	0.59
1:A:6:VAL:HG22	5:A:2000:HOH:O	2.02	0.59
1:A:91:GLU:O	1:A:91:GLU:HG2	2.01	0.59
1:B:514:LYS:HE2	1:B:517:GLU:OE2	2.02	0.59
1:C:910:LEU:HB2	1:C:913:ILE:HD13	1.84	0.59
1:D:1209:TYR:CE2	1:D:1261:LEU:HB2	2.38	0.59
1:A:237:LEU:O	1:A:240:MET:HB3	2.03	0.58
1:B:401:MET:HE3	1:B:748:LEU:HD22	1.85	0.58
1:A:82:ILE:O	1:A:86:VAL:HG23	2.03	0.58
1:A:123:LEU:O	1:A:127:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:LEU:O	1:B:619:VAL:HG11	2.03	0.58
1:A:322:MET:SD	1:B:730:ALA:HB1	2.44	0.58
1:C:1083:GLU:HG2	1:C:1089:SER:OG	2.04	0.58
1:D:1574:VAL:HG13	1:D:1579:GLU:HB3	1.86	0.58
1:A:220:PRO:HA	1:A:357:GLY:O	2.04	0.58
1:A:237:LEU:HB2	5:A:1803:HOH:O	2.03	0.58
1:B:532:GLU:HA	1:B:535:LYS:HE2	1.84	0.58
1:A:256:ILE:HD12	1:A:302:LEU:CD1	2.34	0.58
1:B:404:TRP:HB2	1:B:537:PHE:CE2	2.39	0.58
1:C:1007:ILE:HD11	1:C:1010:LEU:HB2	1.85	0.58
1:C:1021:HIS:CE1	1:C:1158:VAL:HG22	2.39	0.58
1:D:1553:LYS:HE3	1:D:1591:LEU:O	2.04	0.58
1:B:580:SER:O	1:B:584:LEU:HG	2.04	0.58
1:B:652:MET:O	1:B:710:ASP:HA	2.04	0.58
1:A:330:ALA:HB1	1:B:722:MET:SD	2.44	0.57
1:B:654:TYR:OH	1:B:697:GLN:HG3	2.04	0.57
1:B:706:LYS:HD3	1:B:732:ASP:OD2	2.04	0.57
1:C:956:TYR:HE2	1:C:1008:PRO:HD2	1.69	0.57
1:A:275:VAL:O	1:A:278:LYS:HB2	2.04	0.57
1:B:527:VAL:HG23	1:B:528:SER:H	1.69	0.57
1:D:1287:LYS:O	1:D:1291:GLU:HG2	2.04	0.57
1:D:1508:ALA:O	1:D:1527:ILE:HG23	2.04	0.57
1:C:914:LYS:HD2	1:C:918:GLY:O	2.04	0.57
1:D:1352:PRO:HA	1:D:1470:ASN:HA	1.86	0.57
1:D:1515:LYS:HE3	1:D:1519:GLY:CA	2.34	0.57
1:B:551:GLU:HG3	1:B:602:SER:OG	2.05	0.57
1:A:275:VAL:HG13	1:A:294:THR:CG2	2.34	0.57
1:B:406:VAL:HG12	1:B:548:ALA:HB2	1.86	0.57
1:D:1246:TYR:CE1	1:D:1553:LYS:HE2	2.39	0.57
1:D:1280:ARG:O	1:D:1283:LEU:HB3	2.03	0.57
1:A:65:TYR:OH	1:A:69:LYS:HD3	2.05	0.57
1:A:381:PHE:CE1	1:A:385:LYS:HE2	2.39	0.57
1:B:564:LEU:O	1:B:568:GLU:HB2	2.05	0.57
1:A:77:HIS:H	1:A:77:HIS:CD2	2.23	0.57
1:A:235:THR:HG22	1:A:281:VAL:HG11	1.86	0.57
1:C:1076:LEU:O	1:C:1080:LYS:HG3	2.05	0.57
1:D:1350:THR:HG23	1:D:1401:PRO:HD2	1.87	0.57
1:D:1453:SER:HA	1:D:1510:ASP:OD1	2.04	0.57
1:A:168:GLU:O	1:A:171:ILE:HB	2.05	0.57
1:C:1033:VAL:HG22	1:D:1440:MET:HE1	1.86	0.57
1:A:9:TYR:CE2	1:A:61:LEU:HB2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:LYS:HG3	1:B:483:LEU:HD21	1.86	0.56
1:C:1122:MET:SD	1:D:1530:ALA:HB1	2.45	0.56
1:B:458:ILE:HD12	1:B:510:LEU:HD23	1.87	0.56
1:B:616:LYS:HB2	5:B:1924:HOH:O	2.04	0.56
1:D:1353:LEU:HD12	1:D:1473:SER:OG	2.05	0.56
1:A:10:GLY:HA3	5:A:1604:HOH:O	2.05	0.56
1:D:1354:PRO:CB	1:D:1403:PRO:HG3	2.35	0.56
1:B:675:VAL:HG13	1:B:694:THR:CG2	2.36	0.56
1:D:1423:GLY:O	1:D:1424:ASN:HB2	2.03	0.56
1:D:1425:ASP:OD1	1:D:1567:LYS:HE3	2.05	0.56
1:D:1307:ILE:HD13	1:D:1307:ILE:O	2.06	0.56
1:A:101:LEU:HD21	1:A:176:LYS:HB3	1.87	0.56
1:C:806:VAL:HG12	1:C:948:ALA:HB2	1.88	0.56
1:D:1323:LEU:HA	1:D:1326:MET:SD	2.46	0.56
1:B:623:GLY:O	1:B:624:ASN:HB2	2.06	0.56
1:A:131:GLU:HG3	1:A:192:LEU:HD21	1.87	0.56
1:A:104:GLY:CA	1:A:152:PRO:HG3	2.36	0.56
1:C:869:LYS:O	1:C:873:GLU:HG2	2.06	0.56
1:D:1221:ARG:O	1:D:1225:ARG:HB2	2.06	0.56
1:D:1224:GLU:OE2	1:D:1250:SER:HA	2.06	0.56
1:D:1355:ASN:HB2	5:D:1651:HOH:O	2.06	0.56
1:C:1120:LYS:HB2	1:D:1534:ILE:HD13	1.88	0.56
1:A:87:LYS:HG3	1:A:88:SER:N	2.21	0.55
1:A:167:PHE:O	1:A:170:MET:HB3	2.06	0.55
1:C:861:LEU:HD22	1:C:867:ALA:HA	1.88	0.55
1:D:1455:ASN:HD22	1:D:1506:LYS:HZ3	1.52	0.55
1:D:1563:ALA:HB1	1:D:1569:PRO:HB3	1.88	0.55
1:C:804:TRP:NE1	1:C:934:ILE:HG12	2.22	0.55
1:A:230:GLU:CD	1:A:255:ASN:HD21	2.15	0.55
1:B:675:VAL:HG13	1:B:694:THR:HG22	1.88	0.55
1:B:552:PRO:HA	1:B:669:ASP:O	2.06	0.55
1:C:1001:PRO:HG2	1:C:1074:LYS:HB2	1.88	0.55
1:D:1325:GLU:O	1:D:1328:SER:HB3	2.06	0.55
1:D:1531:ILE:HD12	1:D:1531:ILE:H	1.72	0.55
1:A:79:ASP:HB2	1:A:82:ILE:HD12	1.87	0.55
1:B:606:ALA:CB	1:B:624:ASN:HD21	2.18	0.55
1:D:1214:THR:HB	1:D:1268:ALA:HB2	1.89	0.55
1:A:60:LEU:HD13	1:A:97:LYS:CD	2.37	0.55
1:B:402:LYS:HG2	1:B:452:GLU:HB2	1.88	0.55
1:B:457:GLU:O	1:B:497:LYS:HA	2.07	0.55
1:C:802:LYS:HB3	1:C:937:PHE:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1221:ARG:HG2	1:D:1289:ASP:OD1	2.06	0.55
1:D:1456:ILE:O	1:D:1457:LEU:HB3	2.07	0.55
1:D:1331:GLU:O	1:D:1335:LYS:HB3	2.07	0.55
1:D:1431:THR:OG1	1:D:1478:LYS:HB3	2.06	0.55
1:A:225:ASP:O	1:A:366:PHE:HB3	2.06	0.55
1:C:916:LEU:HD13	1:C:921:LEU:HD22	1.88	0.55
1:A:223:GLY:O	1:A:224:ASN:HB2	2.06	0.55
1:B:614:ALA:HB1	1:B:619:VAL:O	2.06	0.55
1:C:1111:PHE:HE2	1:C:1123:LYS:HG2	1.71	0.55
1:C:1150:ALA:O	1:C:1155:VAL:HG23	2.07	0.55
1:D:1217:MET:HB3	1:D:1221:ARG:NH1	2.22	0.55
1:D:1271:HIS:HA	1:D:1274:LEU:HD12	1.89	0.55
1:D:1547:LEU:CD2	1:D:1562:MET:HE1	2.37	0.55
1:A:105:SER:H	1:A:269:ASP:CG	2.15	0.55
1:B:432:GLY:O	1:B:738:PRO:HB2	2.06	0.55
1:C:813:SER:O	1:C:816:ALA:HB3	2.06	0.55
1:C:1153:LYS:HE3	1:C:1191:LEU:O	2.06	0.55
1:A:248:VAL:O	1:A:290:PRO:HB3	2.06	0.54
1:D:1277:HIS:H	1:D:1277:HIS:CD2	2.23	0.54
1:A:268:ARG:HG3	1:A:268:ARG:HH11	1.71	0.54
1:A:173:GLU:HB3	1:A:175:ARG:CD	2.35	0.54
1:B:497:LYS:HE2	1:B:515:THR:HB	1.88	0.54
1:B:510:LEU:CA	1:B:513:ILE:HD12	2.33	0.54
1:B:714:PHE:CE1	1:B:722:MET:HE3	2.43	0.54
1:C:1131:ILE:CB	1:D:1520:LYS:HE2	2.34	0.54
1:A:99:THR:HG22	1:A:185:TYR:CE2	2.42	0.54
5:A:1787:HOH:O	1:B:778:HIS:HB3	2.07	0.54
1:D:1476:LEU:CD2	1:D:1480:LYS:HZ2	2.14	0.54
1:B:513:ILE:O	1:B:514:LYS:HG2	2.07	0.54
1:C:932:GLU:HA	1:C:935:LYS:HD2	1.89	0.54
1:C:1070:ASN:O	1:C:1073:SER:HB2	2.08	0.54
1:D:1331:GLU:HG3	1:D:1388:ALA:CB	2.37	0.54
1:D:1561:GLU:HG2	1:D:1587:TRP:HB2	1.89	0.54
1:D:1567:LYS:CE	2:D:1595:PO4:O4	2.54	0.54
1:C:853:PHE:HB2	1:C:893:ILE:HD13	1.89	0.54
1:C:1153:LYS:CB	1:C:1191:LEU:HD22	2.37	0.54
1:C:805:LEU:HD13	1:C:813:SER:OG	2.08	0.54
1:C:1015:GLU:HG2	1:C:1157:GLY:HA2	1.89	0.54
1:D:1265:TYR:CA	1:D:1290:LEU:HB3	2.37	0.54
1:C:1026:GLY:O	1:C:1167:LYS:HE3	2.08	0.54
1:D:1266:GLU:O	1:D:1269:LYS:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1361:HIS:HB3	1:D:1407:ILE:HD12	1.88	0.54
1:D:1456:ILE:HD12	1:D:1502:LEU:CD1	2.37	0.54
1:B:580:SER:HB3	1:B:583:MET:HG3	1.90	0.54
1:C:1007:ILE:CD1	1:C:1010:LEU:HB2	2.37	0.54
1:D:1407:ILE:CD1	1:D:1409:ALA:HB3	2.38	0.54
1:B:411:ILE:HG12	1:B:733:ALA:CB	2.39	0.53
1:D:1217:MET:HE3	1:D:1253:PHE:CB	2.36	0.53
1:A:299:PHE:HD2	1:C:1093:ILE:HD12	1.73	0.53
1:A:353:LYS:HD2	1:A:391:LEU:O	2.09	0.53
1:C:1054:TYR:OH	1:C:1097:GLN:HG3	2.09	0.53
1:A:108:LYS:O	1:A:109:GLU:HG3	2.08	0.53
1:B:570:MET:O	1:B:570:MET:HG2	2.08	0.53
1:B:695:GLU:HG2	1:B:697:GLN:NE2	2.18	0.53
1:D:1344:VAL:HG11	1:D:1389:ALA:HB2	1.90	0.53
1:A:60:LEU:CD1	1:A:97:LYS:HZ3	2.21	0.53
1:A:298:TYR:CZ	1:A:300:PRO:HB3	2.42	0.53
1:A:365:PHE:HB2	1:A:366:PHE:CE1	2.43	0.53
1:C:944:VAL:HG12	1:C:996:TYR:HD1	1.72	0.53
1:C:944:VAL:HG21	1:C:989:ALA:HB2	1.89	0.53
1:C:1120:LYS:CB	1:D:1534:ILE:HD13	2.38	0.53
1:D:1357:SER:HB3	1:D:1360:TYR:HB2	1.90	0.53
1:A:60:LEU:HB2	1:A:97:LYS:NZ	2.23	0.53
1:A:275:VAL:HG13	1:A:294:THR:HG22	1.90	0.53
1:A:213:LEU:O	1:A:217:LYS:HB2	2.09	0.53
1:B:517:GLU:HB2	1:B:526:MET:CE	2.39	0.53
1:C:899:THR:HA	1:C:916:LEU:HB2	1.90	0.53
1:D:1514:PHE:CE2	1:D:1522:MET:HE3	2.44	0.53
1:A:376:ASN:O	1:A:380:GLN:HG3	2.08	0.53
1:B:412:VAL:CG1	1:B:547:VAL:HG21	2.39	0.53
1:C:1025:ASP:HB3	1:C:1167:LYS:HG3	1.90	0.52
1:D:1456:ILE:HG13	1:D:1507:THR:O	2.09	0.52
1:A:121:LEU:HA	5:A:2050:HOH:O	2.09	0.52
1:A:183:MET:HE2	1:A:207:ILE:HG21	1.92	0.52
1:A:374:VAL:HG12	1:A:380:GLN:HG2	1.91	0.52
1:B:570:MET:HG3	1:B:575:ARG:HB2	1.91	0.52
1:C:809:TYR:HB2	1:C:857:GLU:OE1	2.09	0.52
1:C:1040:MET:HE3	1:D:1436:THR:OG1	2.09	0.52
1:A:276:LEU:O	1:A:280:LYS:HB2	2.10	0.52
1:A:330:ALA:HB2	1:B:722:MET:HB3	1.92	0.52
1:B:421:ARG:HA	1:B:421:ARG:NE	2.24	0.52
1:B:553:LEU:CD1	1:B:672:GLU:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:GLY:HA2	1:B:569:ARG:HD2	1.90	0.52
1:B:748:LEU:HD13	5:B:2108:HOH:O	2.09	0.52
1:C:1027:LYS:HA	1:C:1167:LYS:HE3	1.92	0.52
1:C:916:LEU:HG	1:C:926:MET:SD	2.49	0.52
1:C:931:GLU:O	1:C:935:LYS:HB3	2.08	0.52
1:D:1423:GLY:HA2	1:D:1566:PHE:CE1	2.45	0.52
1:A:60:LEU:HD13	1:A:97:LYS:CE	2.40	0.52
1:A:122:SER:O	1:A:126:MET:HB2	2.10	0.52
1:A:123:LEU:CD1	1:A:176:LYS:HG2	2.39	0.52
1:A:276:LEU:HA	1:A:280:LYS:HE2	1.92	0.52
1:B:654:TYR:HE1	1:B:695:GLU:OE2	1.93	0.52
1:C:1057:LEU:HD13	1:C:1062:GLY:HA2	1.92	0.52
1:D:1559:VAL:HG21	1:D:1562:MET:HE2	1.92	0.52
1:A:153:LEU:HG	1:A:272:GLU:OE1	2.09	0.52
1:B:623:GLY:HA2	1:B:766:PHE:CE1	2.44	0.52
1:D:1420:PRO:HB3	1:D:1555:VAL:HG12	1.91	0.52
1:D:1424:ASN:ND2	1:D:1570:MET:HE3	2.25	0.52
1:A:9:TYR:O	1:A:71:HIS:HE1	1.93	0.52
1:A:228:THR:HG22	1:A:339:LEU:CD1	2.40	0.52
1:C:1139:LEU:O	1:C:1143:ILE:HG13	2.10	0.52
1:D:1306:GLY:C	1:D:1464:VAL:HG13	2.35	0.52
1:A:56:HIS:CE1	1:A:130:ILE:HG23	2.45	0.52
1:A:297:GLN:HG3	1:C:1095:GLU:OE1	2.10	0.52
1:A:376:ASN:HB3	1:A:379:GLU:OE2	2.10	0.52
1:B:417:MET:HE2	1:B:453:PHE:CB	2.37	0.52
1:B:567:PHE:O	1:B:570:MET:HB3	2.09	0.52
1:C:987:TYR:O	1:C:991:LYS:HB2	2.10	0.52
1:D:1435:THR:HA	1:D:1485:MET:CE	2.40	0.52
1:A:115:THR:N	1:A:119:GLU:HB2	2.25	0.51
1:A:127:VAL:HG21	1:A:171:ILE:CD1	2.39	0.51
1:B:509:GLU:HG3	1:B:510:LEU:CD1	2.40	0.51
1:B:631:THR:O	1:B:635:THR:HG23	2.10	0.51
1:B:678:LYS:HE3	2:B:795:PO4:O3	2.08	0.51
1:C:806:VAL:HB	1:C:946:ASN:HA	1.93	0.51
1:C:967:PHE:O	1:C:971:ILE:HD12	2.09	0.51
1:D:1357:SER:CB	1:D:1360:TYR:HB2	2.41	0.51
1:B:423:ILE:HG12	1:B:429:PRO:O	2.11	0.51
1:B:764:PHE:HA	1:B:780:GLN:HB3	1.93	0.51
1:A:190:LEU:HB3	1:A:213:LEU:HD23	1.93	0.51
1:B:514:LYS:HD2	1:B:518:GLY:N	2.25	0.51
1:C:965:GLU:CD	1:C:969:ARG:HH21	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:853:PHE:HB2	1:C:893:ILE:CD1	2.41	0.51
1:C:913:ILE:HG23	1:C:913:ILE:O	2.10	0.51
1:C:935:LYS:HG2	1:C:936:SER:N	2.25	0.51
1:C:947:VAL:O	1:C:947:VAL:HG13	2.10	0.51
1:C:1057:LEU:HD13	1:C:1062:GLY:CA	2.41	0.51
1:D:1354:PRO:HG3	1:D:1403:PRO:HB3	1.92	0.51
1:A:326:PHE:HA	1:B:726:PHE:HA	1.92	0.51
1:B:406:VAL:HG21	1:B:585:TYR:CG	2.46	0.51
1:B:497:LYS:CG	1:B:516:LEU:HD23	2.40	0.51
1:D:1550:ALA:O	1:D:1555:VAL:HB	2.10	0.51
1:A:191:LYS:HE3	5:A:2592:HOH:O	2.11	0.51
1:A:298:TYR:OH	1:A:300:PRO:HB3	2.10	0.51
1:B:635:THR:HA	1:B:685:MET:HE1	1.91	0.51
1:B:779:GLU:O	1:B:783:VAL:HG23	2.11	0.51
1:D:1438:ALA:HB3	1:D:1439:PRO:HD3	1.92	0.51
1:D:1470:ASN:H	1:D:1470:ASN:ND2	2.08	0.51
1:A:169:ARG:O	1:A:173:GLU:HB2	2.10	0.51
1:B:521:LEU:HD23	1:B:525:GLU:HB3	1.93	0.51
1:C:1178:HIS:ND1	1:D:1578:HIS:HB3	2.26	0.51
1:D:1422:ALA:HB2	1:D:1559:VAL:H	1.76	0.51
1:D:1576:ASN:O	1:D:1580:GLN:HG3	2.11	0.51
1:A:173:GLU:HA	1:A:173:GLU:OE2	2.11	0.51
1:D:1550:ALA:HB2	1:D:1587:TRP:HZ2	1.76	0.51
1:B:759:VAL:CG1	1:B:762:MET:HG3	2.41	0.50
1:B:778:HIS:CD2	1:B:778:HIS:H	2.27	0.50
1:C:1111:PHE:CE2	1:C:1123:LYS:HG2	2.46	0.50
1:C:1132:ASP:HB3	3:C:1196:NAD:C7N	2.41	0.50
1:D:1440:MET:O	1:D:1443:TYR:HB2	2.11	0.50
1:D:1448:VAL:O	1:D:1448:VAL:HG12	2.11	0.50
1:A:127:VAL:CG2	1:A:184:LEU:HD22	2.41	0.50
1:B:460:LEU:O	1:B:461:LEU:HD12	2.11	0.50
1:D:1222:ALA:O	1:D:1227:ILE:HG13	2.11	0.50
1:D:1264:ALA:HB3	1:D:1290:LEU:O	2.11	0.50
1:C:860:LEU:HD13	1:C:912:ASP:HB3	1.93	0.50
1:C:1117:PHE:HB3	1:D:1534:ILE:HG23	1.92	0.50
1:A:8:ALA:O	1:A:13:SER:OG	2.29	0.50
1:C:1081:VAL:HG13	1:C:1175:ILE:HG21	1.93	0.50
1:C:1106:LYS:HE2	2:C:1195:PO4:O1	2.11	0.50
1:D:1466:SER:HA	5:D:2015:HOH:O	2.11	0.50
1:A:99:THR:HG22	1:A:185:TYR:CZ	2.47	0.50
1:A:176:LYS:HA	1:A:179:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:LYS:HG2	1:B:536:SER:N	2.27	0.50
1:B:630:GLU:OE2	1:B:710:ASP:OD1	2.30	0.50
1:D:1263:ASN:OD1	1:D:1291:GLU:OE1	2.30	0.50
1:D:1272:TRP:HE1	1:D:1278:PHE:C	2.19	0.50
1:A:97:LYS:HG2	1:A:115:THR:CB	2.38	0.50
1:A:230:GLU:OE1	1:A:310:ASP:OD2	2.29	0.50
1:B:422:ALA:HB1	1:B:428:ALA:HB2	1.94	0.50
1:B:651:TRP:CD2	1:B:712:VAL:HG22	2.47	0.50
1:D:1448:VAL:HG12	1:D:1490:PRO:CB	2.41	0.50
1:D:1563:ALA:CB	1:D:1569:PRO:HB3	2.42	0.50
1:B:675:VAL:HG23	1:B:696:ILE:HD12	1.94	0.50
1:C:880:ARG:O	1:C:884:GLU:OE1	2.30	0.50
1:C:1023:GLY:HA2	1:C:1166:PHE:CE1	2.47	0.50
1:C:1023:GLY:HA2	1:C:1166:PHE:CZ	2.47	0.50
1:D:1344:VAL:O	1:D:1344:VAL:HG12	2.10	0.50
1:A:267:ALA:O	1:A:271:LYS:HB3	2.12	0.50
1:A:21:ARG:O	1:A:25:ARG:HG3	2.11	0.50
1:B:401:MET:CE	1:B:748:LEU:HD22	2.42	0.50
1:D:1351:GLU:HB2	1:D:1352:PRO:HD2	1.94	0.50
1:A:34:VAL:HB	1:A:342:ASP:OD1	2.12	0.49
1:B:402:LYS:HB2	1:B:542:THR:OG1	2.12	0.49
1:C:886:VAL:HG12	1:C:886:VAL:O	2.11	0.49
1:D:1211:ILE:HG12	1:D:1533:ALA:CB	2.42	0.49
1:D:1365:GLU:O	1:D:1369:ARG:HB2	2.12	0.49
1:D:1468:ARG:HA	1:D:1471:LYS:HB3	1.94	0.49
1:D:1591:LEU:O	1:D:1592:LYS:O	2.30	0.49
1:B:547:VAL:O	1:B:547:VAL:HG13	2.12	0.49
1:C:957:SER:O	1:C:961:HIS:HB2	2.12	0.49
1:D:1316:LEU:HD11	1:D:1326:MET:HG2	1.93	0.49
1:A:279:ASP:OD2	1:A:292:SER:OG	2.30	0.49
1:B:516:LEU:HD21	1:B:529:ARG:HD2	1.93	0.49
1:C:965:GLU:HG2	1:C:965:GLU:O	2.10	0.49
1:C:1117:PHE:CG	1:D:1538:PRO:HG3	2.47	0.49
1:D:1328:SER:O	1:D:1332:GLU:OE1	2.30	0.49
1:B:486:VAL:HG12	1:B:490:LEU:HG	1.94	0.49
1:B:515:THR:O	1:B:519:GLU:OE2	2.30	0.49
1:D:1337:PHE:O	1:D:1338:ALA:O	2.30	0.49
1:D:1458:GLY:O	1:D:1459:ASP:O	2.30	0.49
1:A:60:LEU:HD13	1:A:97:LYS:HD2	1.93	0.49
1:B:411:ILE:HG22	3:B:796:NAD:O2N	2.13	0.49
1:B:494:VAL:HG12	1:B:494:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:LYS:HB3	1:B:694:THR:CG2	2.40	0.49
1:B:786:GLU:O	1:B:790:ASN:OD1	2.31	0.49
1:C:858:ILE:HD13	3:C:1196:NAD:C5A	2.42	0.49
1:C:861:LEU:HD22	1:C:867:ALA:CA	2.43	0.49
1:C:1072:GLU:O	1:C:1076:LEU:HG	2.12	0.49
1:C:1056:ILE:HD12	1:C:1102:LEU:CD1	2.43	0.49
1:C:1083:GLU:OE2	1:C:1089:SER:OG	2.30	0.49
1:D:1418:GLY:C	1:D:1556:LYS:HB2	2.37	0.49
1:A:11:ILE:HG13	1:A:71:HIS:CB	2.35	0.49
1:A:134:ILE:O	1:A:138:ALA:HB3	2.13	0.49
1:B:433:LEU:HD21	1:B:741:LEU:HD12	1.94	0.49
1:A:92:GLY:HA3	5:A:1956:HOH:O	2.13	0.49
1:C:1034:LYS:HD3	1:C:1082:LEU:HD13	1.94	0.49
1:A:60:LEU:HD13	1:A:97:LYS:HZ3	1.78	0.49
1:A:96:ARG:CD	1:A:133:ASP:HB3	2.40	0.49
1:A:114:LYS:HG2	1:A:119:GLU:CA	2.40	0.49
1:A:238:ALA:HB3	1:A:239:PRO:HD3	1.94	0.49
1:C:1038:ALA:HB3	1:C:1039:PRO:HD3	1.95	0.49
1:C:1050:GLY:HA2	1:C:1091:TYR:O	2.13	0.49
1:D:1275:ASN:HB2	1:D:1277:HIS:HD2	1.76	0.49
1:D:1347:VAL:HG13	1:D:1347:VAL:O	2.12	0.49
1:A:88:SER:O	1:A:91:GLU:OE2	2.30	0.49
1:C:805:LEU:O	1:C:855:GLY:HA3	2.11	0.49
1:C:1028:THR:HG22	1:C:1139:LEU:HD12	1.95	0.49
1:C:1086:LEU:HB3	1:C:1088:TYR:CE1	2.48	0.49
1:D:1277:HIS:HB2	1:D:1534:ILE:HD11	1.95	0.49
1:D:1334:ILE:HG22	1:D:1392:LEU:HD12	1.95	0.49
1:A:161:HIS:CE1	1:A:170:MET:HE1	2.41	0.48
1:A:249:VAL:HG21	1:A:321:LEU:HD21	1.94	0.48
1:C:802:LYS:HD2	1:C:939:ASP:CG	2.38	0.48
1:C:961:HIS:NE2	1:C:978:TYR:HB3	2.28	0.48
1:D:1506:LYS:HD3	1:D:1532:ASP:OD1	2.13	0.48
1:B:523:LEU:HD21	1:B:579:ALA:CB	2.38	0.48
1:B:711:PHE:CE2	1:B:723:LYS:HB3	2.48	0.48
1:D:1272:TRP:CZ2	1:D:1280:ARG:HB2	2.48	0.48
1:D:1309:GLU:O	1:D:1309:GLU:OE2	2.30	0.48
1:A:132:GLU:O	1:A:136:SER:OG	2.31	0.48
1:A:164:LEU:HD11	1:A:213:LEU:HD12	1.95	0.48
1:A:231:THR:O	1:A:235:THR:HG23	2.13	0.48
1:B:459:ARG:HB2	1:B:510:LEU:HD11	1.94	0.48
1:B:507:ILE:HD13	1:B:508:LYS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1117:PHE:CB	1:D:1538:PRO:HG3	2.42	0.48
1:D:1235:SER:OG	1:D:1542:ASP:OD2	2.30	0.48
1:A:141:GLU:HB3	1:A:348:LEU:HD21	1.96	0.48
1:A:293:ILE:HD11	1:C:1099:PHE:HD2	1.78	0.48
1:A:325:TYR:O	1:B:726:PHE:HB2	2.13	0.48
1:D:1567:LYS:C	1:D:1569:PRO:HD3	2.39	0.48
1:A:224:ASN:O	1:A:366:PHE:HB3	2.14	0.48
1:C:1020:PRO:HD3	1:C:1155:VAL:O	2.13	0.48
1:C:1178:HIS:HB3	1:D:1578:HIS:ND1	2.28	0.48
1:A:33:LEU:HD13	1:A:49:PHE:HE1	1.77	0.48
1:A:196:TYR:CE1	1:A:205:SER:HB3	2.49	0.48
1:B:521:LEU:HD23	1:B:525:GLU:CG	2.43	0.48
1:C:811:ILE:CD1	1:C:871:HIS:HB3	2.42	0.48
1:C:877:HIS:H	1:C:877:HIS:CD2	2.31	0.48
1:C:942:THR:HB	1:C:994:LEU:HD22	1.96	0.48
1:D:1317:GLU:HA	1:D:1317:GLU:OE2	2.13	0.48
1:A:101:LEU:HD12	1:A:126:MET:HE1	1.96	0.48
1:B:515:THR:O	1:B:515:THR:HG22	2.13	0.48
1:D:1346:ASN:HD21	1:D:1400:THR:HG23	1.78	0.48
1:D:1406:ALA:HB2	1:D:1570:MET:HE2	1.95	0.48
1:D:1468:ARG:NH2	1:D:1472:GLU:HG3	2.26	0.48
1:A:116:LEU:HD12	1:A:126:MET:HG2	1.95	0.48
1:A:280:LYS:O	1:A:283:GLU:OE1	2.32	0.48
1:C:903:CYS:HB3	1:C:907:ILE:HD11	1.95	0.48
1:C:1079:ASP:OD2	1:C:1092:SER:OG	2.29	0.48
1:D:1332:GLU:O	1:D:1336:SER:OG	2.30	0.48
1:D:1435:THR:HA	1:D:1485:MET:SD	2.53	0.48
1:B:409:TYR:CG	1:B:457:GLU:HG2	2.49	0.48
1:B:624:ASN:O	1:B:768:SER:HB3	2.14	0.48
1:B:680:LYS:HZ2	1:B:684:LYS:CB	2.22	0.48
1:B:688:TYR:C	1:B:690:PRO:HD3	2.39	0.48
1:D:1474:LYS:HE3	3:D:1596:NAD:C6N	2.43	0.47
1:A:90:LEU:HA	1:A:93:ILE:CD1	2.37	0.47
1:A:106:GLY:C	1:A:264:VAL:HG22	2.40	0.47
1:A:221:HIS:H	1:A:221:HIS:CD2	2.31	0.47
1:B:480:ARG:HD3	1:C:880:ARG:HD2	1.97	0.47
1:D:1396:TYR:CE2	1:D:1405:SER:HB3	2.49	0.47
1:A:61:LEU:HD11	5:A:1999:HOH:O	2.14	0.47
1:A:164:LEU:HD13	1:A:213:LEU:HB2	1.96	0.47
1:B:601:PRO:HG2	1:B:674:LYS:HD2	1.94	0.47
1:B:737:ALA:HB3	1:B:738:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:874:LEU:HB3	1:C:1103:VAL:HG11	1.96	0.47
1:C:899:THR:HB	1:C:916:LEU:CD2	2.42	0.47
1:C:952:PRO:HA	1:C:1070:ASN:HA	1.95	0.47
1:C:958:GLU:HG2	1:C:962:GLY:HA3	1.95	0.47
1:A:280:LYS:HD3	1:A:280:LYS:N	2.29	0.47
1:B:680:LYS:HB2	5:B:2394:HOH:O	2.14	0.47
1:C:957:SER:H	1:C:961:HIS:HD2	1.62	0.47
1:D:1307:ILE:O	1:D:1307:ILE:HG23	2.14	0.47
1:D:1468:ARG:HG2	1:D:1471:LYS:HE2	1.96	0.47
1:A:14:THR:O	1:A:18:VAL:HG23	2.14	0.47
1:B:497:LYS:HG3	1:B:516:LEU:HD23	1.96	0.47
1:B:499:THR:OG1	1:B:517:GLU:HB3	2.15	0.47
1:B:657:LEU:HD13	1:B:662:GLY:CA	2.44	0.47
1:B:710:ASP:HB2	1:B:726:PHE:CZ	2.49	0.47
1:C:1040:MET:HE1	1:D:1433:VAL:CA	2.34	0.47
1:D:1217:MET:O	1:D:1221:ARG:HD2	2.15	0.47
1:D:1386:ALA:HB2	1:D:1396:TYR:CZ	2.49	0.47
1:D:1453:SER:HB3	1:D:1494:THR:HG23	1.97	0.47
1:D:1455:ASN:HD22	1:D:1506:LYS:NZ	2.12	0.47
1:A:58:ILE:HD13	1:A:107:ILE:HD11	1.97	0.47
1:A:107:ILE:HG12	1:A:107:ILE:O	2.14	0.47
1:B:445:LYS:HB3	1:B:446:TYR:CE1	2.49	0.47
1:C:811:ILE:O	1:C:815:THR:OG1	2.30	0.47
1:C:864:ALA:HB3	1:C:893:ILE:HB	1.95	0.47
1:D:1582:VAL:O	1:D:1586:GLU:HG3	2.15	0.47
1:A:260:TYR:CA	1:A:263:LYS:HG3	2.42	0.47
1:C:835:SER:OG	1:C:1142:ASP:OD2	2.30	0.47
1:C:1152:LYS:HE2	5:C:1801:HOH:O	2.13	0.47
1:C:1172:THR:OG1	1:C:1174:VAL:HG23	2.15	0.47
1:D:1304:GLY:HA3	1:D:1307:ILE:HG21	1.96	0.47
1:D:1460:TYR:HB3	3:D:1596:NAD:O1A	2.15	0.47
1:A:19:GLY:HA2	1:B:718:LEU:HD21	1.97	0.47
1:A:44:GLU:O	1:A:48:PRO:HD3	2.14	0.47
1:B:402:LYS:HD3	1:B:537:PHE:O	2.14	0.47
1:B:411:ILE:HD11	1:B:477:HIS:NE2	2.30	0.47
1:B:421:ARG:HA	1:B:421:ARG:HE	1.80	0.47
1:B:470:GLU:HG2	1:B:471:HIS:N	2.29	0.47
1:B:553:LEU:HD13	1:B:672:GLU:HB3	1.97	0.47
1:C:1126:PHE:HB2	1:D:1525:TYR:O	2.15	0.47
1:A:317:PHE:O	1:A:318:LEU:HB2	2.14	0.47
1:C:982:SER:O	1:C:1004:GLY:HA2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:NH1	1:A:133:ASP:OD1	2.48	0.47
1:B:405:LEU:HD13	1:B:413:SER:OG	2.14	0.47
1:D:1461:ASP:O	1:D:1465:LEU:HG	2.15	0.47
1:C:859:ARG:NH1	1:C:861:LEU:HD11	2.30	0.46
1:C:1120:LYS:HG2	1:D:1534:ILE:HD13	1.97	0.46
1:D:1370:MET:HG2	1:D:1371:ILE:N	2.29	0.46
1:A:254:TYR:HD2	1:A:295:GLU:HB2	1.80	0.46
1:D:1452:MET:O	1:D:1510:ASP:HA	2.14	0.46
1:A:61:LEU:HD12	1:A:67:ALA:CB	2.42	0.46
1:A:320:LYS:HD2	1:A:321:LEU:N	2.30	0.46
1:B:701:SER:HB2	1:D:1449:VAL:HG12	1.97	0.46
1:B:782:VAL:O	1:B:785:LYS:HB2	2.14	0.46
1:C:932:GLU:HG2	1:C:935:LYS:NZ	2.30	0.46
1:C:1084:LYS:H	1:C:1084:LYS:HG3	1.47	0.46
1:D:1586:GLU:O	1:D:1589:SER:HB2	2.15	0.46
1:A:219:VAL:HG12	1:A:220:PRO:HD2	1.97	0.46
1:B:725:TYR:O	1:B:726:PHE:HB3	2.15	0.46
1:C:908:LYS:O	1:C:909:GLU:HG2	2.15	0.46
1:A:223:GLY:HA3	1:A:366:PHE:CE1	2.51	0.46
1:A:374:VAL:CG1	1:A:379:GLU:HB3	2.45	0.46
1:B:623:GLY:HA2	1:B:766:PHE:CZ	2.51	0.46
1:B:628:THR:O	1:B:629:GLY:O	2.32	0.46
1:C:1018:GLY:HA2	1:C:1156:LYS:HB2	1.97	0.46
1:D:1415:GLU:OE1	1:D:1415:GLU:HA	2.15	0.46
1:A:255:ASN:OD1	1:A:308:ALA:HB2	2.16	0.46
1:A:280:LYS:HA	1:A:283:GLU:OE1	2.15	0.46
1:D:1206:VAL:HG21	1:D:1385:TYR:CG	2.49	0.46
1:D:1221:ARG:HE	1:D:1289:ASP:HB3	1.81	0.46
1:A:195:PRO:HD3	1:A:351:LYS:HE3	1.97	0.46
1:C:947:VAL:O	3:C:1196:NAD:H51N	2.15	0.46
1:D:1201:MET:O	1:D:1252:GLU:OE2	2.34	0.46
1:D:1422:ALA:HB2	1:D:1559:VAL:N	2.30	0.46
1:B:463:ASN:ND2	1:B:491:GLU:HG3	2.31	0.46
1:D:1437:LEU:O	1:D:1437:LEU:HG	2.16	0.46
1:B:423:ILE:HG12	1:B:428:ALA:O	2.15	0.46
1:B:463:ASN:OD1	1:B:465:TYR:HB3	2.16	0.46
1:C:950:THR:HG21	1:C:1065:LEU:HD21	1.97	0.46
1:A:2:LYS:HB2	1:A:142:THR:OG1	2.16	0.45
1:A:247:GLU:HG2	1:A:315:LYS:HD3	1.98	0.45
1:B:480:ARG:CD	1:C:880:ARG:HD2	2.45	0.45
1:B:551:GLU:HG3	1:B:602:SER:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1064:VAL:O	1:C:1070:ASN:ND2	2.49	0.45
1:D:1547:LEU:HD21	1:D:1562:MET:HE1	1.97	0.45
1:A:114:LYS:HG3	1:A:118:GLY:O	2.17	0.45
1:A:134:ILE:HD11	1:A:194:LEU:HD12	1.98	0.45
1:A:196:TYR:O	1:A:221:HIS:HA	2.16	0.45
1:B:514:LYS:HE2	1:B:517:GLU:CG	2.47	0.45
1:C:804:TRP:CE2	1:C:934:ILE:HG12	2.51	0.45
1:C:903:CYS:HA	1:C:952:PRO:HD2	1.98	0.45
1:C:1051:TRP:CD2	1:C:1112:VAL:HG22	2.51	0.45
1:D:1314:LYS:HD3	1:D:1318:GLY:HA2	1.98	0.45
1:D:1406:ALA:HA	1:D:1570:MET:HE2	1.97	0.45
1:D:1558:VAL:HG11	1:D:1570:MET:HB3	1.97	0.45
1:D:1577:THR:HA	1:D:1580:GLN:HG3	1.99	0.45
1:A:149:SER:H	3:A:396:NAD:H8A	1.81	0.45
1:B:501:LEU:HA	1:B:517:GLU:OE1	2.17	0.45
1:B:560:TYR:CE2	1:B:569:ARG:HD3	2.51	0.45
1:B:628:THR:OG1	1:B:629:GLY:N	2.49	0.45
1:B:774:VAL:C	1:B:775:ILE:HD13	2.41	0.45
1:C:809:TYR:O	1:C:871:HIS:HE1	1.99	0.45
1:C:822:ALA:O	1:C:827:ILE:HB	2.17	0.45
1:A:173:GLU:OE1	1:A:175:ARG:NH1	2.50	0.45
1:B:461:LEU:HB3	1:B:462:SER:H	1.65	0.45
1:B:527:VAL:O	1:B:530:ILE:N	2.50	0.45
1:B:583:MET:HE2	1:B:607:ILE:CD1	2.42	0.45
1:C:916:LEU:HD11	1:C:926:MET:HB3	1.89	0.45
1:C:1044:ARG:NH1	1:D:1539:LEU:HD11	2.32	0.45
1:C:1091:TYR:HE1	1:C:1093:ILE:HD11	1.81	0.45
1:C:1171:ASP:N	1:C:1171:ASP:OD1	2.50	0.45
1:D:1368:GLU:OE2	1:D:1391:LYS:NZ	2.50	0.45
1:D:1398:ASN:ND2	1:D:1400:THR:O	2.50	0.45
1:D:1542:ASP:O	1:D:1546:PHE:HD1	1.99	0.45
1:A:376:ASN:O	1:A:379:GLU:HB2	2.16	0.45
1:B:459:ARG:HG3	1:B:510:LEU:HD12	1.97	0.45
1:C:941:GLU:HB3	1:C:1148:LEU:HD21	1.97	0.45
1:C:1105:ASN:HA	1:C:1131:ILE:HD13	1.97	0.45
1:D:1539:LEU:N	1:D:1539:LEU:HD23	2.31	0.45
1:A:60:LEU:O	1:A:61:LEU:HD23	2.16	0.45
1:A:243:TYR:OH	1:A:376:ASN:ND2	2.50	0.45
1:B:466:GLU:OE1	1:B:469:LYS:NZ	2.50	0.45
1:B:469:LYS:HG3	1:B:483:LEU:CD2	2.47	0.45
1:C:1104:ASP:O	1:C:1106:LYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1412:GLU:OE2	1:D:1412:GLU:N	2.50	0.45
1:A:110:LEU:O	1:A:112:ASP:N	2.50	0.45
1:A:115:THR:O	1:A:129:ARG:NH1	2.50	0.45
1:A:228:THR:HG22	1:A:339:LEU:HD12	1.99	0.45
1:B:446:TYR:O	1:B:752:LYS:NZ	2.50	0.45
1:B:487:LYS:NZ	1:B:491:GLU:OE2	2.50	0.45
1:B:499:THR:N	1:B:585:TYR:OH	2.50	0.45
1:C:1014:ALA:O	1:C:1018:GLY:N	2.50	0.45
1:C:1167:LYS:C	1:C:1169:PRO:HD3	2.42	0.45
1:D:1206:VAL:HG12	1:D:1348:ALA:HB2	1.99	0.45
1:B:409:TYR:HE2	1:B:461:LEU:N	2.08	0.45
1:B:452:GLU:OE2	1:B:452:GLU:N	2.50	0.45
1:D:1406:ALA:CA	1:D:1570:MET:HE2	2.47	0.45
1:D:1468:ARG:NH2	1:D:1472:GLU:OE1	2.50	0.45
1:A:235:THR:HG22	1:A:281:VAL:CG1	2.46	0.45
1:C:959:GLU:N	1:C:959:GLU:OE2	2.50	0.45
1:D:1244:GLU:H	1:D:1244:GLU:CD	2.24	0.45
1:D:1354:PRO:O	1:D:1356:TYR:N	2.50	0.45
1:D:1360:TYR:O	1:D:1367:PHE:N	2.50	0.45
1:D:1365:GLU:O	1:D:1369:ARG:N	2.50	0.45
1:B:483:LEU:O	1:B:487:LYS:N	2.50	0.45
1:D:1474:LYS:HE2	1:D:1567:LYS:NZ	2.25	0.45
1:A:153:LEU:HD23	1:A:273:SER:OG	2.17	0.44
1:B:656:ILE:HD12	1:B:702:LEU:CD1	2.46	0.44
1:B:680:LYS:NZ	1:B:680:LYS:O	2.50	0.44
1:D:1277:HIS:HB2	1:D:1534:ILE:CD1	2.47	0.44
1:D:1472:GLU:O	1:D:1476:LEU:HG	2.17	0.44
1:A:110:LEU:HD13	1:A:113:ILE:HG21	1.98	0.44
1:D:1345:ILE:O	1:D:1345:ILE:HG22	2.15	0.44
1:A:105:SER:HB2	1:A:269:ASP:OD2	2.17	0.44
1:A:199:PHE:HZ	1:A:339:LEU:HD12	1.82	0.44
1:C:857:GLU:HG3	1:C:859:ARG:H	1.82	0.44
1:C:921:LEU:HD21	1:C:929:ARG:HH12	1.78	0.44
1:C:968:GLU:OE2	1:C:991:LYS:NZ	2.50	0.44
1:C:1007:ILE:HG12	1:C:1010:LEU:H	1.83	0.44
1:C:1078:LYS:HB2	1:C:1078:LYS:HE3	1.76	0.44
1:D:1300:ALA:O	1:D:1301:LEU:HG	2.18	0.44
1:D:1357:SER:OG	1:D:1360:TYR:N	2.50	0.44
1:D:1400:THR:O	1:D:1425:ASP:N	2.50	0.44
1:A:24:GLU:OE2	1:A:51:PHE:N	2.49	0.44
1:A:214:ALA:O	1:A:218:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:GLY:N	5:B:1774:HOH:O	2.50	0.44
1:B:539:ASP:OD2	1:B:542:THR:N	2.51	0.44
1:B:560:TYR:HD2	1:B:566:GLY:O	2.00	0.44
1:B:627:LYS:HD2	1:B:632:LEU:HA	1.99	0.44
1:C:935:LYS:NZ	5:C:1857:HOH:O	2.50	0.44
1:D:1290:LEU:HD12	1:D:1290:LEU:HA	1.71	0.44
1:D:1334:ILE:O	1:D:1337:PHE:N	2.51	0.44
1:D:1504:ASP:O	1:D:1506:LYS:N	2.50	0.44
1:B:402:LYS:HB3	1:B:542:THR:HG23	2.00	0.44
1:B:497:LYS:HG2	1:B:516:LEU:HD23	2.00	0.44
1:B:600:THR:HG1	1:B:602:SER:H	1.65	0.44
1:C:944:VAL:HG12	1:C:996:TYR:CD1	2.52	0.44
1:C:997:ALA:HB2	1:C:1147:LEU:HD11	1.98	0.44
1:D:1265:TYR:HA	1:D:1290:LEU:HB3	2.00	0.44
1:D:1396:TYR:CD2	1:D:1405:SER:HB3	2.53	0.44
1:A:268:ARG:NH2	5:A:1891:HOH:O	2.50	0.44
1:A:320:LYS:HD2	1:A:321:LEU:H	1.83	0.44
1:A:349:PHE:O	1:A:353:LYS:HG2	2.18	0.44
1:C:807:GLY:HA2	3:C:1196:NAD:N3A	2.31	0.44
1:C:997:ALA:HA	1:C:1022:ALA:O	2.18	0.44
1:C:1030:GLU:OE2	1:C:1053:SER:HB3	2.18	0.44
1:C:1065:LEU:O	1:C:1071:LYS:HB2	2.16	0.44
1:C:1152:LYS:HE2	5:C:2065:HOH:O	2.17	0.44
1:A:22:ALA:HB2	1:A:82:ILE:HG23	1.98	0.44
1:A:150:THR:HG22	1:A:270:ASN:HB3	1.99	0.44
1:B:723:LYS:NZ	1:D:1529:ASP:OD2	2.50	0.44
1:C:881:GLU:H	1:C:881:GLU:HG3	1.45	0.44
1:C:1011:LYS:HE2	1:C:1170:MET:HE2	1.99	0.44
1:C:1056:ILE:HD12	1:C:1102:LEU:HD11	1.98	0.44
1:C:1085:MET:O	1:C:1086:LEU:HD23	2.17	0.44
1:C:1160:LYS:HE2	1:C:1171:ASP:CB	2.47	0.44
1:C:1169:PRO:HB2	1:C:1172:THR:CG2	2.48	0.44
1:B:649:VAL:HG21	1:B:721:LEU:CD2	2.48	0.44
1:D:1209:TYR:CD2	1:D:1257:GLU:HG2	2.53	0.44
1:D:1428:THR:CG2	3:D:1596:NAD:H4N	2.48	0.44
1:A:144:VAL:HG21	1:A:189:ALA:HB2	2.00	0.44
1:B:567:PHE:HB2	1:B:609:ALA:HB1	1.99	0.44
1:A:101:LEU:HD22	1:A:179:ALA:O	2.18	0.43
1:A:149:SER:OG	3:A:396:NAD:H8A	2.18	0.43
1:A:289:SER:HB3	5:A:2049:HOH:O	2.17	0.43
1:A:311:PHE:CZ	1:A:323:LYS:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:VAL:O	1:A:386:GLU:HB2	2.18	0.43
1:B:427:ILE:HG23	1:B:427:ILE:O	2.16	0.43
1:B:621:HIS:O	1:B:622:ALA:HB2	2.17	0.43
1:C:815:THR:HB	1:C:1137:ALA:HB2	2.00	0.43
1:D:1217:MET:HE3	1:D:1253:PHE:CG	2.53	0.43
1:D:1289:ASP:O	1:D:1292:GLY:N	2.50	0.43
1:D:1303:CYS:O	1:D:1352:PRO:HG3	2.17	0.43
1:A:203:PRO:O	1:A:206:ALA:HB3	2.18	0.43
1:B:649:VAL:HG23	1:B:713:HIS:O	2.19	0.43
1:D:1233:LEU:HB2	1:D:1236:GLU:HB2	1.99	0.43
1:D:1346:ASN:ND2	1:D:1400:THR:HG23	2.34	0.43
1:A:9:TYR:CD2	1:A:57:GLU:HG3	2.53	0.43
1:A:260:TYR:O	1:A:263:LYS:HB2	2.19	0.43
1:B:425:ARG:NH2	1:B:489:ASP:OD1	2.51	0.43
1:C:995:PRO:HA	1:C:1019:VAL:CG1	2.47	0.43
1:C:1057:LEU:N	1:C:1057:LEU:HD12	2.33	0.43
1:D:1204:TRP:HE1	1:D:1256:HIS:CE1	2.36	0.43
1:D:1248:PRO:O	1:D:1250:SER:N	2.50	0.43
1:A:172:ASP:OD2	1:A:172:ASP:N	2.50	0.43
1:B:514:LYS:HE2	1:B:517:GLU:HG2	2.00	0.43
1:B:534:ILE:O	1:B:538:ALA:HB2	2.18	0.43
1:B:783:VAL:HG11	5:B:1724:HOH:O	2.18	0.43
1:C:872:TRP:O	1:C:876:ARG:N	2.51	0.43
1:C:903:CYS:SG	1:C:951:GLU:HB2	2.58	0.43
1:C:969:ARG:O	1:C:973:GLU:N	2.50	0.43
1:C:1040:MET:HE3	1:D:1436:THR:CB	2.48	0.43
1:C:1105:ASN:CA	1:C:1131:ILE:HD13	2.48	0.43
1:D:1211:ILE:O	1:D:1215:THR:OG1	2.30	0.43
1:D:1517:PHE:O	1:D:1518:LEU:HB2	2.19	0.43
1:D:1559:VAL:CB	1:D:1562:MET:HE2	2.49	0.43
1:A:68:ALA:HA	5:A:1919:HOH:O	2.18	0.43
1:A:241:PHE:CZ	1:A:312:VAL:HG11	2.53	0.43
1:B:638:ALA:HB3	1:B:639:PRO:HD3	2.01	0.43
1:D:1345:ILE:CD1	1:D:1544:ALA:HB2	2.49	0.43
1:D:1410:LEU:HD22	1:D:1410:LEU:HA	1.83	0.43
1:D:1481:VAL:HG12	1:D:1482:LEU:N	2.33	0.43
1:D:1549:PHE:CZ	1:D:1591:LEU:HB2	2.54	0.43
1:C:1132:ASP:OD1	1:C:1132:ASP:N	2.50	0.43
1:C:1140:ILE:N	1:C:1140:ILE:HD13	2.32	0.43
1:D:1240:PHE:O	1:D:1243:ILE:HG22	2.19	0.43
1:D:1421:HIS:O	1:D:1422:ALA:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1436:THR:O	1:D:1436:THR:HG22	2.19	0.43
1:D:1484:LYS:HE2	1:D:1573:ASN:OD1	2.19	0.43
1:D:1518:LEU:N	1:D:1518:LEU:HD23	2.33	0.43
1:B:676:LEU:HD23	1:B:676:LEU:HA	1.75	0.43
1:B:701:SER:HB2	1:D:1449:VAL:CG1	2.48	0.43
1:B:759:VAL:HG12	1:B:762:MET:HG3	2.00	0.43
1:C:841:GLU:H	1:C:841:GLU:HG3	1.59	0.43
1:C:1020:PRO:HB3	1:C:1155:VAL:HG12	2.01	0.43
1:C:1068:ARG:O	1:C:1072:GLU:HB2	2.19	0.43
1:D:1559:VAL:HB	1:D:1562:MET:HE2	2.01	0.43
1:A:167:PHE:CD2	1:A:170:MET:HE2	2.54	0.43
1:A:265:LEU:HD23	1:A:271:LYS:HG3	2.01	0.43
1:D:1233:LEU:O	1:D:1236:GLU:HB2	2.18	0.43
1:D:1243:ILE:HD12	1:D:1588:TYR:HE1	1.84	0.43
1:D:1316:LEU:HD11	1:D:1326:MET:CG	2.47	0.43
1:D:1360:TYR:CZ	1:D:1375:ARG:HG3	2.54	0.43
1:A:151:GLU:HG2	1:A:152:PRO:HD2	2.01	0.43
1:B:498:GLY:O	1:B:499:THR:HB	2.19	0.43
1:B:547:VAL:CG2	3:B:796:NAD:H51N	2.44	0.43
1:C:913:ILE:O	1:C:915:THR:N	2.50	0.43
1:C:1068:ARG:O	1:C:1068:ARG:HG2	2.19	0.43
1:D:1429:GLY:HA3	1:D:1528:TRP:CZ2	2.54	0.43
1:A:89:ASP:OD2	1:A:89:ASP:N	2.50	0.42
1:A:369:PRO:HB2	1:A:372:THR:HG22	2.00	0.42
1:C:901:LEU:HD21	1:C:976:LYS:HD3	2.01	0.42
1:C:977:GLU:H	1:C:977:GLU:HG3	1.64	0.42
1:D:1555:VAL:HG22	5:D:2272:HOH:O	2.18	0.42
1:D:1559:VAL:CG2	1:D:1562:MET:HE2	2.48	0.42
1:A:20:ALA:O	1:A:24:GLU:N	2.49	0.42
1:A:42:GLY:O	1:A:45:LYS:HG3	2.18	0.42
1:B:465:TYR:OH	1:B:487:LYS:HE2	2.19	0.42
1:D:1491:TYR:HE2	1:D:1493:ILE:HD11	1.84	0.42
1:A:41:GLU:HB3	5:A:2354:HOH:O	2.19	0.42
1:B:559:GLU:OE1	1:B:569:ARG:NH1	2.50	0.42
1:B:773:ASN:O	1:B:775:ILE:HD13	2.18	0.42
1:C:901:LEU:H	1:C:981:ALA:HB2	1.84	0.42
1:C:1023:GLY:HA2	1:C:1166:PHE:CD1	2.54	0.42
1:C:1030:GLU:HB3	2:C:1195:PO4:O3	2.19	0.42
1:A:13:SER:OG	1:A:14:THR:N	2.52	0.42
1:A:73:GLU:O	1:A:73:GLU:HG3	2.19	0.42
1:A:257:LEU:HD21	1:A:261:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ILE:HG13	1:B:477:HIS:HE2	1.84	0.42
1:C:1122:MET:HB3	1:D:1530:ALA:HB2	2.01	0.42
1:A:302:LEU:O	1:A:303:VAL:HB	2.19	0.42
1:A:379:GLU:O	1:A:383:VAL:HG23	2.19	0.42
1:B:410:GLY:O	1:B:414:THR:HG23	2.20	0.42
1:B:720:LYS:HD2	1:B:720:LYS:HA	1.46	0.42
1:C:927:VAL:O	1:C:931:GLU:HB2	2.19	0.42
1:C:984:LEU:O	1:C:988:ALA:HB2	2.19	0.42
1:C:1019:VAL:HA	1:C:1020:PRO:HD2	1.84	0.42
1:C:1060:TYR:HA	1:C:1063:LYS:HB2	2.00	0.42
1:C:1134:ILE:CG1	1:D:1520:LYS:HD3	2.38	0.42
1:D:1583:VAL:HG12	1:D:1584:LEU:N	2.35	0.42
1:B:500:ALA:HB2	3:B:796:NAD:N6A	2.34	0.42
1:B:758:VAL:CG1	1:B:770:MET:HB2	2.48	0.42
1:C:921:LEU:HD23	1:C:926:MET:HG2	2.01	0.42
1:B:483:LEU:O	1:B:487:LYS:HB2	2.19	0.42
1:B:747:LEU:HA	1:B:747:LEU:HD23	1.69	0.42
1:C:1034:LYS:O	1:C:1085:MET:HE1	2.19	0.42
1:D:1548:LEU:O	1:D:1552:LYS:HG3	2.19	0.42
1:A:259:ASP:HB3	1:A:261:ASP:OD1	2.19	0.42
1:A:285:MET:HE2	1:A:285:MET:HB2	1.76	0.42
1:B:704:ASP:O	1:B:706:LYS:N	2.51	0.42
1:B:711:PHE:HE2	1:B:723:LYS:HB3	1.84	0.42
1:C:960:TYR:HE2	1:C:969:ARG:HH11	1.66	0.42
1:C:960:TYR:OH	1:C:975:ARG:NE	2.50	0.42
1:C:1139:LEU:N	1:C:1139:LEU:HD23	2.34	0.42
1:D:1442:ALA:HA	5:D:1620:HOH:O	2.20	0.42
1:D:1484:LYS:HB3	1:D:1484:LYS:HE3	1.72	0.42
1:D:1506:LYS:N	1:D:1530:ALA:O	2.53	0.42
1:A:17:MET:O	1:A:20:ALA:HB3	2.20	0.42
1:B:406:VAL:HG21	1:B:585:TYR:CD1	2.54	0.42
1:B:412:VAL:HG11	1:B:547:VAL:HG21	2.02	0.42
1:C:1131:ILE:CG2	1:C:1134:ILE:HD13	2.50	0.42
1:D:1224:GLU:CD	1:D:1250:SER:HA	2.45	0.42
1:D:1468:ARG:HG2	1:D:1468:ARG:HH11	1.85	0.42
1:D:1575:ILE:HA	1:D:1580:GLN:HE21	1.85	0.42
1:A:39:HIS:CD2	1:A:385:LYS:HG2	2.55	0.42
1:A:244:ARG:HB3	1:A:246:MET:HE2	2.01	0.42
1:A:372:THR:HG23	1:A:373:ASN:N	2.34	0.42
1:B:501:LEU:HD12	1:B:523:LEU:HD11	2.02	0.42
1:B:598:ASN:ND2	1:B:602:SER:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:954:PRO:HG3	1:C:1003:PRO:HG2	2.01	0.42
1:D:1316:LEU:CD2	1:D:1326:MET:HG2	2.35	0.42
1:D:1553:LYS:HD2	1:D:1553:LYS:HA	1.74	0.42
1:B:501:LEU:HD23	1:B:501:LEU:HA	1.89	0.41
1:C:960:TYR:OH	1:C:975:ARG:NH2	2.50	0.41
1:D:1316:LEU:HD11	1:D:1326:MET:SD	2.59	0.41
1:D:1455:ASN:ND2	1:D:1506:LYS:NZ	2.68	0.41
1:C:871:HIS:HE2	1:C:1060:TYR:HE1	1.64	0.41
1:D:1206:VAL:O	1:D:1348:ALA:HB2	2.20	0.41
1:A:276:LEU:N	1:A:276:LEU:HD23	2.35	0.41
1:A:303:VAL:HG12	1:A:304:ASP:N	2.35	0.41
1:B:446:TYR:CE2	1:B:753:LYS:HE2	2.56	0.41
1:B:501:LEU:HD21	5:B:2404:HOH:O	2.20	0.41
1:B:648:VAL:HG21	1:B:686:LEU:HD11	2.01	0.41
1:C:945:ILE:HG12	1:C:997:ALA:HB3	2.02	0.41
1:C:1024:ASN:O	1:C:1168:SER:HB2	2.20	0.41
1:D:1539:LEU:O	1:D:1543:ILE:HD12	2.19	0.41
1:A:123:LEU:CD2	1:A:184:LEU:HD11	2.50	0.41
1:B:465:TYR:HB2	1:B:490:LEU:HB2	2.02	0.41
1:B:510:LEU:C	1:B:513:ILE:HD12	2.46	0.41
1:B:678:LYS:O	1:B:694:THR:OG1	2.32	0.41
1:B:739:LEU:N	1:B:739:LEU:HD23	2.35	0.41
1:B:750:ALA:HB1	1:B:755:VAL:HB	2.02	0.41
1:C:1084:LYS:HB3	1:C:1173:ASN:ND2	2.16	0.41
1:D:1476:LEU:HB3	1:D:1480:LYS:HZ2	1.84	0.41
1:A:90:LEU:HA	1:A:90:LEU:HD22	1.90	0.41
1:A:378:HIS:HB3	5:A:1787:HOH:O	2.19	0.41
1:C:857:GLU:OE2	3:C:1196:NAD:H1B	2.21	0.41
1:D:1366:GLY:O	1:D:1369:ARG:N	2.50	0.41
1:D:1465:LEU:HB3	1:D:1471:LYS:HG3	2.02	0.41
1:D:1532:ASP:CB	3:D:1596:NAD:H72N	2.25	0.41
1:A:9:TYR:CD2	1:A:61:LEU:HB2	2.56	0.41
1:B:775:ILE:HD13	1:B:775:ILE:N	2.35	0.41
1:C:997:ALA:HB2	1:C:1147:LEU:CD1	2.51	0.41
1:D:1246:TYR:HD1	1:D:1549:PHE:HD2	1.69	0.41
1:D:1329:ARG:CA	1:D:1332:GLU:HB2	2.49	0.41
1:A:235:THR:HB	1:A:375:ILE:O	2.21	0.41
1:A:314:PHE:CE2	1:A:322:MET:HE3	2.56	0.41
1:C:923:LEU:HD12	1:C:923:LEU:HA	1.85	0.41
1:A:57:GLU:OE2	3:A:396:NAD:O3B	2.30	0.41
1:A:116:LEU:HB3	1:A:117:GLU:H	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TYR:O	1:A:308:ALA:HA	2.21	0.41
1:A:299:PHE:CD2	1:C:1093:ILE:HD12	2.54	0.41
1:A:340:ILE:N	1:A:340:ILE:HD13	2.35	0.41
5:A:2516:HOH:O	1:D:1280:ARG:HG2	2.21	0.41
1:B:564:LEU:HB2	1:B:609:ALA:O	2.21	0.41
1:C:990:LEU:HD22	1:C:1014:ALA:CB	2.44	0.41
1:D:1482:LEU:HD23	1:D:1490:PRO:HG2	2.03	0.41
1:D:1550:ALA:HB2	1:D:1587:TRP:CZ2	2.55	0.41
1:A:1:MET:N	1:A:50:SER:O	2.50	0.41
1:A:15:THR:O	1:A:15:THR:HG22	2.20	0.41
1:A:142:THR:O	1:A:143:VAL:HG13	2.20	0.41
1:A:142:THR:HG22	1:A:143:VAL:N	2.36	0.41
1:B:647:GLU:HG3	1:B:648:VAL:N	2.32	0.41
1:C:859:ARG:HG3	1:C:910:LEU:CD1	2.35	0.41
1:C:1018:GLY:HA2	1:C:1156:LYS:CB	2.51	0.41
1:C:1040:MET:CE	1:D:1432:LEU:HG	2.45	0.41
1:C:1089:SER:HA	1:C:1090:PRO:HD2	1.94	0.41
1:D:1256:HIS:HA	1:D:1296:ARG:O	2.20	0.41
1:D:1259:ARG:CG	1:D:1310:LEU:HG	2.45	0.41
1:D:1377:GLU:HG3	5:D:2346:HOH:O	2.21	0.41
1:A:57:GLU:OE2	3:A:396:NAD:H1B	2.20	0.41
1:A:130:ILE:O	1:A:130:ILE:HG22	2.20	0.41
1:A:164:LEU:HD11	1:A:213:LEU:CD1	2.51	0.41
1:A:315:LYS:HG2	1:A:321:LEU:CD2	2.51	0.41
1:B:480:ARG:HH11	1:B:480:ARG:HG2	1.86	0.41
1:D:1204:TRP:CE2	1:D:1255:GLY:HA2	2.56	0.41
1:D:1257:GLU:OE1	3:D:1596:NAD:O3B	2.39	0.41
1:D:1304:GLY:HA3	1:D:1307:ILE:CG2	2.51	0.41
1:D:1406:ALA:CB	1:D:1570:MET:HE2	2.50	0.41
1:D:1508:ALA:O	1:D:1527:ILE:HA	2.20	0.41
1:A:205:SER:OG	1:A:370:MET:HE1	2.21	0.40
1:B:411:ILE:HA	1:B:414:THR:OG1	2.21	0.40
1:B:610:LEU:HD12	1:B:610:LEU:HA	1.89	0.40
1:B:615:GLU:OE1	1:B:615:GLU:HA	2.20	0.40
1:A:11:ILE:HD13	1:A:333:ALA:CB	2.47	0.40
1:A:216:LYS:O	1:A:216:LYS:HG3	2.21	0.40
1:A:239:PRO:HB3	1:A:243:TYR:CZ	2.57	0.40
1:B:418:VAL:HG22	1:B:490:LEU:HD11	2.03	0.40
1:B:428:ALA:HA	1:B:429:PRO:HD3	1.93	0.40
1:B:551:GLU:O	1:B:673:SER:OG	2.30	0.40
1:B:627:LYS:H	1:B:766:PHE:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:ARG:O	1:B:672:GLU:N	2.50	0.40
1:B:671:LYS:HE2	1:B:675:VAL:CG2	2.46	0.40
1:B:704:ASP:HA	5:B:2522:HOH:O	2.20	0.40
1:C:804:TRP:CD2	1:C:855:GLY:HA2	2.56	0.40
1:C:849:PHE:CE1	1:C:851:PHE:HE1	2.39	0.40
1:D:1358:GLU:H	1:D:1358:GLU:HG3	1.59	0.40
1:A:252:MET:HE2	1:A:309:PHE:O	2.21	0.40
1:A:309:PHE:CE2	1:C:1052:MET:HE1	2.57	0.40
1:B:412:VAL:HG22	1:B:733:ALA:HA	2.03	0.40
1:B:532:GLU:O	1:B:532:GLU:HG2	2.21	0.40
1:B:740:ILE:N	1:B:740:ILE:HD13	2.35	0.40
1:C:954:PRO:CG	1:C:1003:PRO:HG2	2.51	0.40
1:C:1131:ILE:HB	1:C:1134:ILE:HD13	2.03	0.40
1:D:1407:ILE:HD11	1:D:1409:ALA:HB3	2.03	0.40
1:A:110:LEU:CB	1:A:113:ILE:HB	2.52	0.40
1:A:228:THR:HG22	1:A:339:LEU:HD11	2.03	0.40
1:B:539:ASP:OD2	1:B:542:THR:OG1	2.30	0.40
1:B:782:VAL:O	1:B:786:GLU:HG3	2.21	0.40
1:C:815:THR:OG1	1:C:1133:ALA:HB1	2.21	0.40
1:C:994:LEU:O	1:C:1019:VAL:HG11	2.22	0.40
1:D:1310:LEU:O	1:D:1313:ILE:HB	2.21	0.40
1:D:1326:MET:HB2	1:D:1326:MET:HE2	1.73	0.40
1:A:281:VAL:HG13	1:A:375:ILE:HG21	2.04	0.40
1:B:507:ILE:HG22	5:B:1774:HOH:O	2.22	0.40
1:B:698:TYR:O	1:D:1493:ILE:HD11	2.21	0.40
1:C:897:LYS:NZ	1:C:919:GLU:OE1	2.55	0.40
1:C:1035:THR:HA	1:C:1085:MET:HE1	2.04	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	390/392 (100%)	343 (88%)	36 (9%)	11 (3%)	4	0
1	B	390/392 (100%)	331 (85%)	43 (11%)	16 (4%)	2	0
1	C	390/392 (100%)	340 (87%)	37 (10%)	13 (3%)	3	0
1	D	390/392 (100%)	324 (83%)	43 (11%)	23 (6%)	1	0
All	All	1560/1568 (100%)	1338 (86%)	159 (10%)	63 (4%)	2	0

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	115	THR
1	A	224	ASN
1	B	505	SER
1	B	629	GLY
1	B	717	PHE
1	C	1024	ASN
1	C	1073	SER
1	C	1117	PHE
1	D	1262	SER
1	D	1302	ASN
1	D	1338	ALA
1	D	1339	ASP
1	D	1459	ASP
1	A	111	GLY
1	A	269	ASP
1	A	303	VAL
1	A	333	ALA
1	B	509	GLU
1	B	511	GLY
1	C	909	GLU
1	C	916	LEU
1	C	1164	PHE
1	D	1303	CYS
1	D	1355	ASN
1	D	1424	ASN
1	D	1505	ASN
1	D	1558	VAL
1	A	104	GLY
1	B	501	LEU
1	C	908	LYS
1	C	963	SER
1	C	1025	ASP

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Mol	Chain	Res	Type
1	C	1105	ASN
1	D	1287	LYS
1	D	1320	GLY
1	D	1429	GLY
1	D	1469	ASP
1	B	514	LYS
1	B	603	PRO
1	B	624	ASN
1	B	703	VAL
1	B	705	ASN
1	C	1103	VAL
1	D	1457	LEU
1	D	1503	VAL
1	A	106	GLY
1	A	107	ILE
1	B	429	PRO
1	C	913	ILE
1	C	1029	GLY
1	D	1307	ILE
1	D	1376	LYS
1	D	1425	ASP
1	B	681	VAL
1	D	1289	ASP
1	B	498	GLY
1	D	1583	VAL
1	B	658	GLY
1	A	220	PRO
1	D	1559	VAL
1	B	774	VAL
1	D	1366	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	325/325 (100%)	238 (73%)	87 (27%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	325/325 (100%)	246 (76%)	79 (24%)	1	0
1	C	325/325 (100%)	255 (78%)	70 (22%)	1	0
1	D	325/325 (100%)	238 (73%)	87 (27%)	0	0
All	All	1300/1300 (100%)	977 (75%)	323 (25%)	1	0

All (323) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	13	SER
1	A	21	ARG
1	A	27	ILE
1	A	30	LYS
1	A	31	ILE
1	A	35	SER
1	A	45	LYS
1	A	59	ARG
1	A	66	GLU
1	A	69	LYS
1	A	76	ARG
1	A	77	HIS
1	A	80	ARG
1	A	81	GLU
1	A	87	LYS
1	A	88	SER
1	A	89	ASP
1	A	90	LEU
1	A	91	GLU
1	A	96	ARG
1	A	97	LYS
1	A	101	LEU
1	A	105	SER
1	A	107	ILE
1	A	108	LYS
1	A	110	LEU
1	A	113	ILE
1	A	114	LYS
1	A	116	LEU
1	A	117	GLU
1	A	121	LEU
1	A	125	GLU

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Mol	Chain	Res	Type
1	A	126	MET
1	A	128	SER
1	A	132	GLU
1	A	134	ILE
1	A	136	SER
1	A	150	THR
1	A	151	GLU
1	A	157	SER
1	A	158	GLU
1	A	165	GLU
1	A	170	MET
1	A	172	ASP
1	A	173	GLU
1	A	174	ASP
1	A	175	ARG
1	A	180	SER
1	A	191	LYS
1	A	202	SER
1	A	215	GLU
1	A	217	LYS
1	A	219	VAL
1	A	221	HIS
1	A	232	LEU
1	A	247	GLU
1	A	249	VAL
1	A	256	ILE
1	A	257	LEU
1	A	261	ASP
1	A	265	LEU
1	A	268	ARG
1	A	274	LYS
1	A	277	SER
1	A	280	LYS
1	A	281	VAL
1	A	285	MET
1	A	286	LEU
1	A	289	SER
1	A	292	SER
1	A	293	ILE
1	A	294	THR
1	A	306	LYS
1	A	315	LYS

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Mol	Chain	Res	Type
1	A	317	PHE
1	A	323	LYS
1	A	334	ILE
1	A	340	ILE
1	A	348	LEU
1	A	360	LYS
1	A	372	THR
1	A	377	THR
1	A	380	GLN
1	A	382	VAL
1	A	384	LEU
1	A	389	SER
1	B	411	ILE
1	B	412	VAL
1	B	427	ILE
1	B	431	ILE
1	B	443	ILE
1	B	445	LYS
1	B	458	ILE
1	B	469	LYS
1	B	474	LEU
1	B	477	HIS
1	B	481	GLU
1	B	482	ILE
1	B	484	GLU
1	B	488	SER
1	B	490	LEU
1	B	491	GLU
1	B	496	ARG
1	B	497	LYS
1	B	499	THR
1	B	501	LEU
1	B	507	ILE
1	B	508	LYS
1	B	514	LYS
1	B	516	LEU
1	B	517	GLU
1	B	521	LEU
1	B	523	LEU
1	B	527	VAL
1	B	528	SER
1	B	529	ARG

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Mol	Chain	Res	Type
1	B	531	GLU
1	B	534	ILE
1	B	535	LYS
1	B	537	PHE
1	B	540	ASP
1	B	541	GLU
1	B	544	VAL
1	B	565	GLU
1	B	569	ARG
1	B	571	ILE
1	B	577	GLU
1	B	600	THR
1	B	610	LEU
1	B	612	GLU
1	B	615	GLU
1	B	616	LYS
1	B	635	THR
1	B	637	LEU
1	B	640	MET
1	B	641	PHE
1	B	653	SER
1	B	656	ILE
1	B	657	LEU
1	B	672	GLU
1	B	674	LYS
1	B	677	SER
1	B	678	LYS
1	B	682	LEU
1	B	683	GLU
1	B	684	LYS
1	B	689	SER
1	B	693	ILE
1	B	701	SER
1	B	706	LYS
1	B	707	THR
1	B	720	LYS
1	B	725	TYR
1	B	731	ILE
1	B	734	ILE
1	B	735	VAL
1	B	747	LEU
1	B	748	LEU

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Mol	Chain	Res	Type
1	B	760	LYS
1	B	773	ASN
1	B	775	ILE
1	B	777	THR
1	B	778	HIS
1	B	782	VAL
1	B	792	LYS
1	C	806	VAL
1	C	812	VAL
1	C	818	VAL
1	C	823	ILE
1	C	827	ILE
1	C	831	ILE
1	C	841	GLU
1	C	843	ILE
1	C	845	LYS
1	C	846	TYR
1	C	858	ILE
1	C	860	LEU
1	C	861	LEU
1	C	869	LYS
1	C	877	HIS
1	C	879	ASP
1	C	880	ARG
1	C	881	GLU
1	C	890	LEU
1	C	891	GLU
1	C	901	LEU
1	C	903	CYS
1	C	905	SER
1	C	907	ILE
1	C	908	LYS
1	C	912	ASP
1	C	914	LYS
1	C	916	LEU
1	C	917	GLU
1	C	921	LEU
1	C	923	LEU
1	C	925	GLU
1	C	932	GLU
1	C	935	LYS
1	C	940	ASP

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Mol	Chain	Res	Type
1	C	947	VAL
1	C	949	SER
1	C	951	GLU
1	C	957	SER
1	C	963	SER
1	C	971	ILE
1	C	972	ASP
1	C	977	GLU
1	C	980	SER
1	C	1002	SER
1	C	1007	ILE
1	C	1016	LYS
1	C	1046	MET
1	C	1047	GLU
1	C	1057	LEU
1	C	1059	ASP
1	C	1063	LYS
1	C	1064	VAL
1	C	1068	ARG
1	C	1069	ASP
1	C	1070	ASN
1	C	1071	LYS
1	C	1073	SER
1	C	1077	SER
1	C	1082	LEU
1	C	1084	LYS
1	C	1095	GLU
1	C	1101	SER
1	C	1110	ASP
1	C	1151	LYS
1	C	1167	LYS
1	C	1170	MET
1	C	1171	ASP
1	C	1175	ILE
1	C	1192	LYS
1	D	1202	LYS
1	D	1213	SER
1	D	1227	ILE
1	D	1231	ILE
1	D	1235	SER
1	D	1241	GLU
1	D	1250	SER

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Mol	Chain	Res	Type
1	D	1252	GLU
1	D	1253	PHE
1	D	1262	SER
1	D	1269	LYS
1	D	1274	LEU
1	D	1276	ARG
1	D	1277	HIS
1	D	1280	ARG
1	D	1286	VAL
1	D	1287	LYS
1	D	1290	LEU
1	D	1303	CYS
1	D	1307	ILE
1	D	1308	LYS
1	D	1309	GLU
1	D	1310	LEU
1	D	1313	ILE
1	D	1314	LYS
1	D	1316	LEU
1	D	1321	LEU
1	D	1323	LEU
1	D	1326	MET
1	D	1332	GLU
1	D	1333	ASP
1	D	1335	LYS
1	D	1336	SER
1	D	1345	ILE
1	D	1346	ASN
1	D	1358	GLU
1	D	1365	GLU
1	D	1370	MET
1	D	1371	ILE
1	D	1372	ASP
1	D	1376	LYS
1	D	1377	GLU
1	D	1380	SER
1	D	1383	MET
1	D	1384	LEU
1	D	1400	THR
1	D	1402	SER
1	D	1410	LEU
1	D	1412	GLU

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Mol	Chain	Res	Type
1	D	1415	GLU
1	D	1416	LYS
1	D	1424	ASN
1	D	1427	LYS
1	D	1430	GLU
1	D	1437	LEU
1	D	1453	SER
1	D	1456	ILE
1	D	1457	LEU
1	D	1466	SER
1	D	1469	ASP
1	D	1470	ASN
1	D	1474	LYS
1	D	1477	SER
1	D	1478	LYS
1	D	1480	LYS
1	D	1483	GLU
1	D	1484	LYS
1	D	1486	LEU
1	D	1495	GLU
1	D	1496	ILE
1	D	1497	GLN
1	D	1512	VAL
1	D	1522	MET
1	D	1534	ILE
1	D	1535	VAL
1	D	1541	LEU
1	D	1551	LYS
1	D	1556	LYS
1	D	1558	VAL
1	D	1559	VAL
1	D	1560	LYS
1	D	1567	LYS
1	D	1568	SER
1	D	1575	ILE
1	D	1579	GLU
1	D	1580	GLN
1	D	1589	SER

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	71	HIS
1	A	77	HIS
1	A	102	ASN
1	A	155	ASN
1	A	161	HIS
1	A	297	GLN
1	B	624	ASN
1	B	697	GLN
1	C	839	HIS
1	C	946	ASN
1	C	955	ASN
1	C	1055	ASN
1	C	1097	GLN
1	C	1173	ASN
1	D	1271	HIS
1	D	1277	HIS
1	D	1302	ASN
1	D	1346	ASN
1	D	1355	ASN
1	D	1361	HIS
1	D	1398	ASN
1	D	1424	ASN
1	D	1455	ASN
1	D	1470	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAD	B	796	4	46,48,48	1.63	7 (15%)	64,73,73	1.08	5 (7%)
2	PO4	D	1595	-	4,4,4	0.95	0	6,6,6	0.52	0
3	NAD	D	1596	-	46,48,48	1.50	7 (15%)	64,73,73	1.04	6 (9%)
3	NAD	C	1196	4	46,48,48	1.52	7 (15%)	64,73,73	1.12	6 (9%)
2	PO4	B	795	-	4,4,4	0.95	0	6,6,6	0.51	0
2	PO4	C	1195	-	4,4,4	0.96	0	6,6,6	0.52	0
2	PO4	A	395	-	4,4,4	0.90	0	6,6,6	0.50	0
3	NAD	A	396	-	46,48,48	2.10	8 (17%)	64,73,73	1.14	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	396	-	-	8/30/62/62	0/5/5/5
3	NAD	D	1596	-	-	1/30/62/62	0/5/5/5
3	NAD	B	796	4	-	1/30/62/62	0/5/5/5
3	NAD	C	1196	4	-	8/30/62/62	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	396	NAD	C3N-C7N	-8.78	1.37	1.50
3	D	1596	NAD	C2N-N1N	6.83	1.42	1.35
3	A	396	NAD	C2N-N1N	6.79	1.42	1.35
3	C	1196	NAD	C2N-N1N	6.50	1.42	1.35
3	B	796	NAD	C2N-N1N	6.49	1.42	1.35
3	A	396	NAD	C2N-C3N	5.05	1.47	1.39
3	B	796	NAD	PA-O3	-4.25	1.54	1.59
3	B	796	NAD	PN-O3	-3.55	1.55	1.59
3	C	1196	NAD	PA-O3	-2.85	1.56	1.59
3	D	1596	NAD	C2A-N1A	2.68	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	396	NAD	C6N-N1N	2.68	1.41	1.35
3	C	1196	NAD	C2A-N1A	2.67	1.38	1.33
3	A	396	NAD	C2A-N1A	2.64	1.38	1.33
3	B	796	NAD	C2A-N1A	2.61	1.38	1.33
3	A	396	NAD	C7N-N7N	2.60	1.37	1.33
3	B	796	NAD	C6N-N1N	2.56	1.41	1.35
3	C	1196	NAD	C6N-N1N	2.53	1.41	1.35
3	D	1596	NAD	C6N-N1N	2.49	1.41	1.35
3	C	1196	NAD	O4B-C1B	-2.37	1.36	1.42
3	D	1596	NAD	PA-O3	-2.34	1.57	1.59
3	B	796	NAD	O4B-C1B	-2.24	1.36	1.42
3	C	1196	NAD	PN-O3	-2.22	1.57	1.59
3	C	1196	NAD	C7N-N7N	2.17	1.37	1.33
3	D	1596	NAD	C7N-N7N	2.15	1.36	1.33
3	B	796	NAD	C7N-N7N	2.14	1.36	1.33
3	D	1596	NAD	O4B-C1B	-2.14	1.37	1.42
3	A	396	NAD	O4B-C1B	-2.12	1.37	1.42
3	D	1596	NAD	O4D-C1D	2.08	1.43	1.40
3	A	396	NAD	PN-O3	-2.02	1.57	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	396	NAD	C5N-C4N-C3N	3.96	124.26	120.36
3	C	1196	NAD	O7N-C7N-C3N	-3.80	114.95	119.60
3	B	796	NAD	O7N-C7N-C3N	-3.76	115.00	119.60
3	D	1596	NAD	O4D-C4D-C5D	3.03	119.03	109.33
3	D	1596	NAD	O4B-C1B-C2B	-2.99	100.22	106.62
3	C	1196	NAD	C4D-O4D-C1D	-2.84	107.32	109.92
3	A	396	NAD	C3N-C7N-N7N	-2.79	114.30	117.74
3	B	796	NAD	O4B-C1B-C2B	-2.71	100.82	106.62
3	C	1196	NAD	C2B-C3B-C4B	-2.67	97.46	102.61
3	A	396	NAD	O4D-C4D-C5D	2.62	117.72	109.33
3	B	796	NAD	O2A-PA-O3	2.56	114.19	107.27
3	C	1196	NAD	C2N-C3N-C4N	2.53	121.19	118.26
3	B	796	NAD	C2N-C3N-C4N	2.51	121.18	118.26
3	D	1596	NAD	C2B-C3B-C4B	-2.35	98.07	102.61
3	B	796	NAD	O2N-PN-O3	2.33	113.57	107.27
3	D	1596	NAD	O7N-C7N-C3N	-2.31	116.77	119.60
3	C	1196	NAD	O4B-C1B-C2B	-2.26	101.78	106.62
3	A	396	NAD	C2B-C3B-C4B	-2.25	98.26	102.61
3	D	1596	NAD	O5B-C5B-C4B	-2.25	101.34	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	396	NAD	C6N-N1N-C2N	-2.20	120.00	121.88
3	A	396	NAD	O5B-C5B-C4B	-2.19	101.53	108.99
3	A	396	NAD	O4B-C1B-C2B	-2.16	101.99	106.62
3	D	1596	NAD	C6N-N1N-C2N	-2.11	120.08	121.88
3	C	1196	NAD	C6N-N1N-C2N	-2.01	120.17	121.88

There are no chirality outliers.

All (18) torsion outliers are listed below:

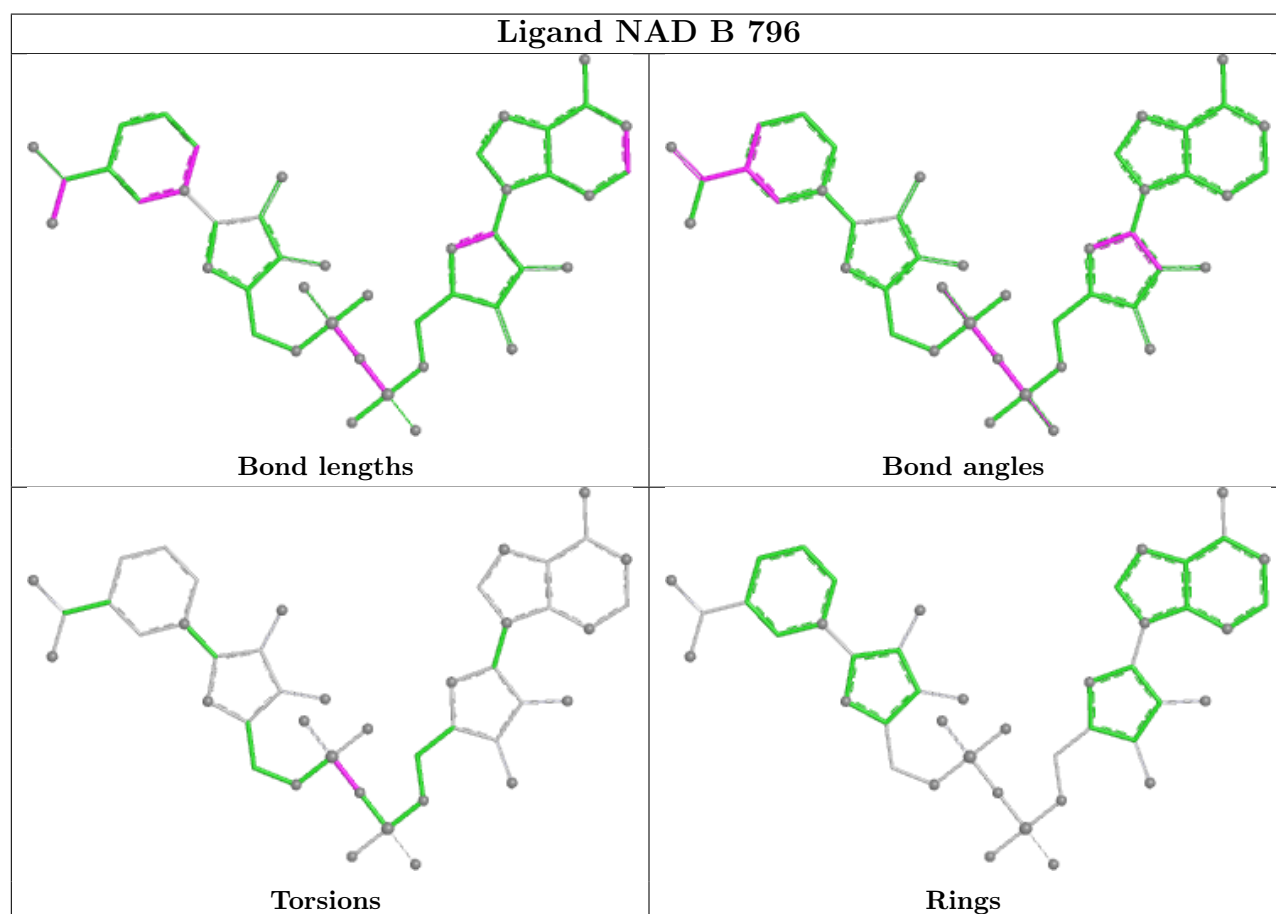
Mol	Chain	Res	Type	Atoms
3	A	396	NAD	O4D-C1D-N1N-C2N
3	A	396	NAD	O4D-C1D-N1N-C6N
3	A	396	NAD	C2D-C1D-N1N-C2N
3	A	396	NAD	C2D-C1D-N1N-C6N
3	C	1196	NAD	C5B-O5B-PA-O1A
3	C	1196	NAD	C5B-O5B-PA-O3
3	A	396	NAD	C3B-C4B-C5B-O5B
3	A	396	NAD	O4B-C4B-C5B-O5B
3	C	1196	NAD	C3B-C4B-C5B-O5B
3	A	396	NAD	O4D-C4D-C5D-O5D
3	C	1196	NAD	O4B-C4B-C5B-O5B
3	C	1196	NAD	C2B-C1B-N9A-C8A
3	C	1196	NAD	C5B-O5B-PA-O2A
3	B	796	NAD	PA-O3-PN-O2N
3	C	1196	NAD	PA-O3-PN-O1N
3	C	1196	NAD	PA-O3-PN-O2N
3	D	1596	NAD	O4B-C4B-C5B-O5B
3	A	396	NAD	PA-O3-PN-O2N

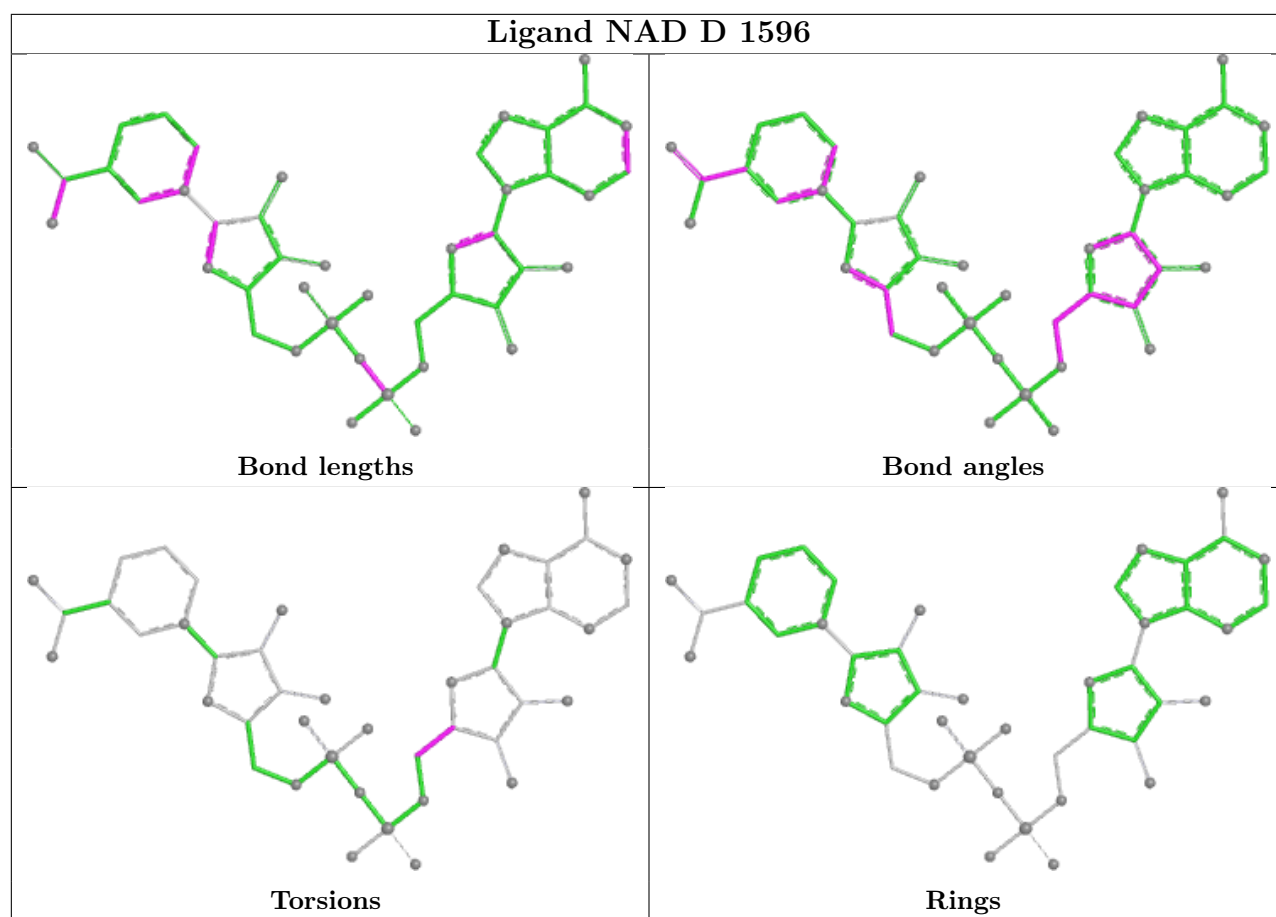
There are no ring outliers.

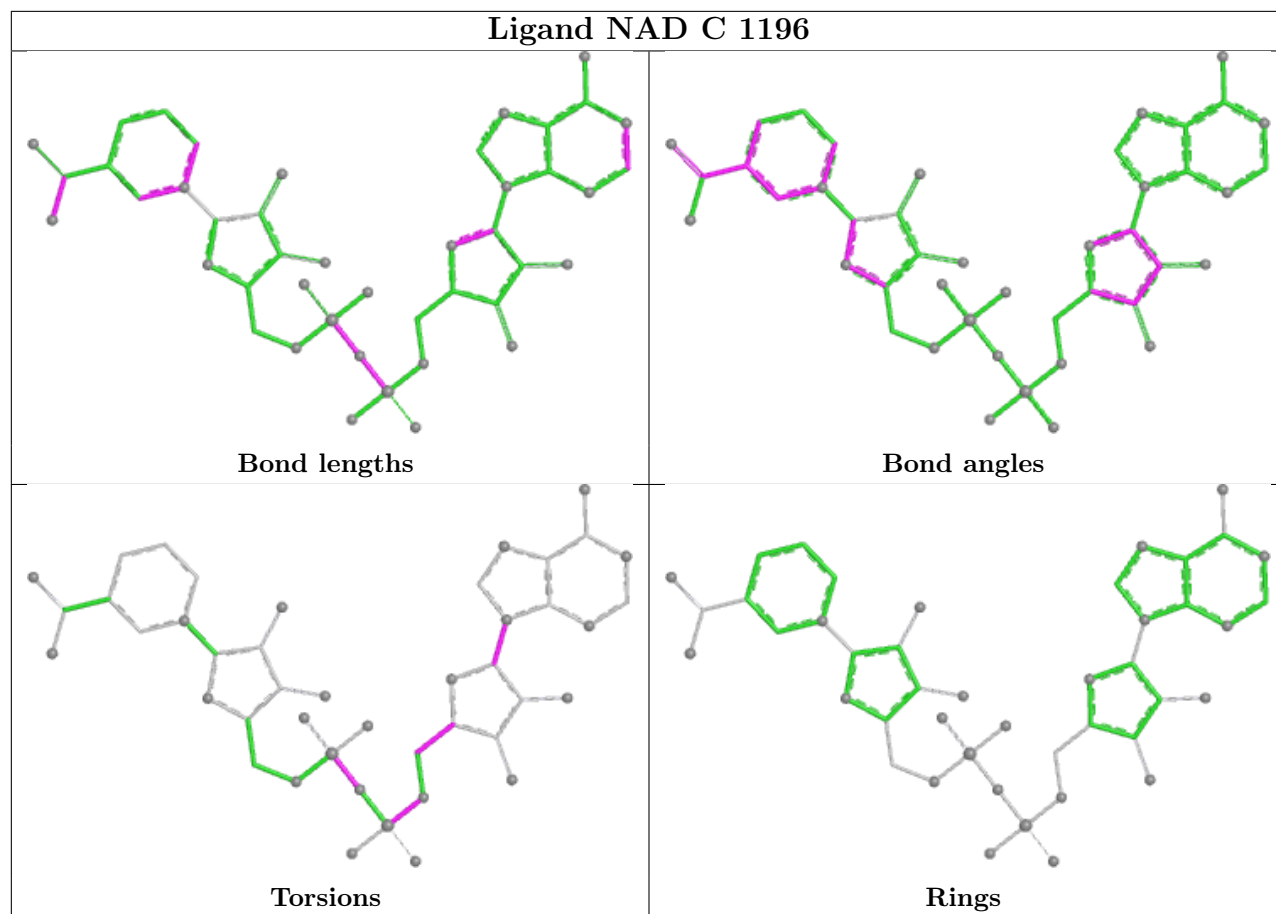
8 monomers are involved in 34 short contacts:

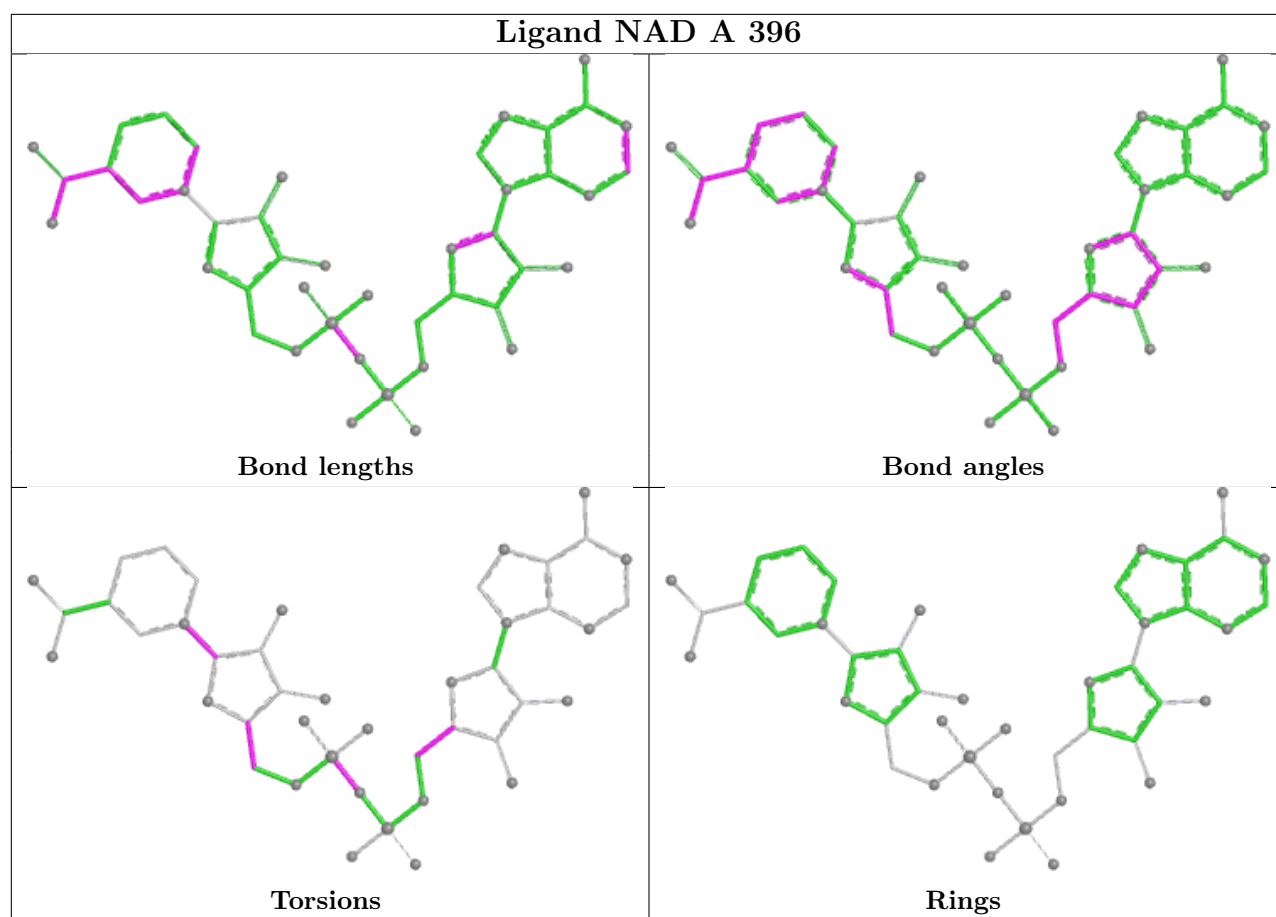
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	796	NAD	5	0
2	D	1595	PO4	2	0
3	D	1596	NAD	9	0
3	C	1196	NAD	8	0
2	B	795	PO4	1	0
2	C	1195	PO4	2	0
2	A	395	PO4	1	0
3	A	396	NAD	6	0

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 [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	392/392 (100%)	1.14	56 (14%) 6 6	14, 41, 77, 131	0
1	B	392/392 (100%)	1.13	63 (16%) 4 4	16, 42, 80, 158	0
1	C	392/392 (100%)	1.04	52 (13%) 7 7	7, 38, 71, 131	0
1	D	392/392 (100%)	1.16	62 (15%) 5 5	14, 43, 80, 149	0
All	All	1568/1568 (100%)	1.12	233 (14%) 5 6	7, 41, 77, 158	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	910	LEU	5.9
1	C	906	GLY	5.7
1	C	1059	ASP	5.5
1	A	116	LEU	5.5
1	B	506	GLY	5.2
1	A	134	ILE	4.9
1	B	516	LEU	4.8
1	B	623	GLY	4.7
1	B	614	ALA	4.7
1	B	507	ILE	4.7
1	C	916	LEU	4.6
1	C	907	ILE	4.5
1	D	1315	THR	4.4
1	D	1357	SER	4.3
1	D	1307	ILE	4.2
1	A	223	GLY	4.0
1	B	667	ALA	4.0
1	D	1364	LEU	3.9
1	D	1347	VAL	3.9
1	C	886	VAL	3.9
1	D	1344	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	658	GLY	3.9
1	D	1316	LEU	3.8
1	A	258	GLY	3.7
1	C	903	CYS	3.7
1	A	201	PRO	3.7
1	C	1067	ALA	3.7
1	B	490	LEU	3.6
1	C	1060	TYR	3.6
1	C	1023	GLY	3.6
1	C	911	GLY	3.6
1	D	1371	ILE	3.5
1	D	1267	ALA	3.5
1	C	1007	ILE	3.5
1	A	375	ILE	3.5
1	A	213	LEU	3.5
1	A	107	ILE	3.4
1	D	1313	ILE	3.4
1	C	954	PRO	3.3
1	B	660	TYR	3.2
1	D	1407	ILE	3.2
1	B	557	SER	3.2
1	A	124	ALA	3.2
1	B	669	ASP	3.2
1	D	1462	GLY	3.1
1	B	458	ILE	3.1
1	D	1310	LEU	3.1
1	A	103	CYS	3.1
1	B	460	LEU	3.1
1	D	1260	LEU	3.1
1	C	1000	THR	3.1
1	A	10	GLY	3.1
1	B	513	ILE	3.0
1	A	160	TYR	3.0
1	B	674	LYS	3.0
1	D	1209	TYR	3.0
1	C	1009	ALA	3.0
1	A	260	TYR	3.0
1	A	264	VAL	3.0
1	A	179	ALA	3.0
1	C	1058	GLY	3.0
1	D	1362	GLY	3.0
1	A	11	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	431	ILE	2.9
1	A	164	LEU	2.9
1	B	675	VAL	2.9
1	A	113	ILE	2.8
1	A	276	LEU	2.8
1	C	1024	ASN	2.8
1	D	1282	ILE	2.8
1	A	32	GLY	2.8
1	B	501	LEU	2.8
1	B	635	THR	2.8
1	B	582	SER	2.8
1	B	514	LYS	2.8
1	D	1311	GLY	2.8
1	D	1290	LEU	2.8
1	C	1075	VAL	2.8
1	B	548	ALA	2.7
1	A	111	GLY	2.7
1	B	566	GLY	2.7
1	A	123	LEU	2.7
1	C	1065	LEU	2.7
1	D	1464	VAL	2.7
1	D	1272	TRP	2.7
1	D	1302	ASN	2.7
1	B	504	GLY	2.7
1	D	1422	ALA	2.7
1	B	560	TYR	2.7
1	C	915	THR	2.7
1	B	665	LEU	2.7
1	B	624	ASN	2.7
1	C	827	ILE	2.7
1	A	120	GLY	2.6
1	A	337	ALA	2.6
1	B	649	VAL	2.6
1	D	1560	LYS	2.6
1	C	899	THR	2.6
1	C	955	ASN	2.6
1	B	472	TRP	2.6
1	A	110	LEU	2.6
1	D	1413	LEU	2.6
1	D	1591	LEU	2.6
1	B	659	ASP	2.6
1	A	282	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	686	LEU	2.5
1	C	912	ASP	2.5
1	C	1004	GLY	2.5
1	A	189	ALA	2.5
1	C	950	THR	2.5
1	C	1008	PRO	2.5
1	B	511	GLY	2.5
1	B	549	SER	2.5
1	D	1264	ALA	2.5
1	D	1449	VAL	2.5
1	D	1312	ASP	2.5
1	C	901	LEU	2.5
1	D	1258	ILE	2.5
1	B	509	GLU	2.5
1	A	115	THR	2.5
1	D	1303	CYS	2.4
1	C	978	TYR	2.4
1	B	739	LEU	2.4
1	D	1359	GLU	2.4
1	C	1002	SER	2.4
1	A	20	ALA	2.4
1	B	508	LYS	2.4
1	B	589	ALA	2.4
1	A	162	GLY	2.4
1	B	503	CYS	2.4
1	B	676	LEU	2.4
1	B	617	LYS	2.4
1	D	1350	THR	2.4
1	C	938	ALA	2.4
1	D	1389	ALA	2.4
1	D	1476	LEU	2.3
1	D	1588	TYR	2.3
1	A	95	ALA	2.3
1	B	775	ILE	2.3
1	C	913	ILE	2.3
1	C	898	GLY	2.3
1	D	1242	GLY	2.3
1	A	86	VAL	2.3
1	A	72	TRP	2.3
1	B	588	ALA	2.3
1	B	717	PHE	2.3
1	B	505	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	680	LYS	2.3
1	A	138	ALA	2.2
1	B	428	ALA	2.2
1	B	478	PHE	2.2
1	B	597	ALA	2.2
1	B	662	GLY	2.2
1	C	846	TYR	2.2
1	D	1506	LYS	2.2
1	B	480	ARG	2.2
1	B	629	GLY	2.2
1	D	1423	GLY	2.2
1	A	267	ALA	2.2
1	B	404	TRP	2.2
1	C	1054	TYR	2.2
1	D	1337	PHE	2.2
1	B	534	ILE	2.2
1	A	170	MET	2.2
1	D	1558	VAL	2.2
1	A	228	THR	2.2
1	C	1177	THR	2.2
1	D	1384	LEU	2.2
1	C	966	GLY	2.2
1	D	1477	SER	2.2
1	C	995	PRO	2.2
1	A	363	ALA	2.2
1	A	178	TYR	2.2
1	C	960	TYR	2.2
1	C	1080	LYS	2.2
1	D	1256	HIS	2.2
1	C	1049	VAL	2.2
1	A	61	LEU	2.2
1	A	153	LEU	2.2
1	A	262	GLY	2.2
1	A	354	GLY	2.2
1	B	687	GLY	2.2
1	B	719	GLY	2.2
1	A	47	ALA	2.2
1	B	609	ALA	2.2
1	A	156	TYR	2.1
1	A	187	TYR	2.1
1	D	1246	TYR	2.1
1	D	1488	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	147	VAL	2.1
1	D	1475	VAL	2.1
1	D	1306	GLY	2.1
1	A	348	LEU	2.1
1	C	953	LEU	2.1
1	D	1375	ARG	2.1
1	D	1401	PRO	2.1
1	C	1006	ALA	2.1
1	A	270	ASN	2.1
1	A	302	LEU	2.1
1	B	564	LEU	2.1
1	B	642	ALA	2.1
1	D	1406	ALA	2.1
1	C	949	SER	2.1
1	A	119	GLU	2.1
1	C	917	GLU	2.1
1	B	426	GLY	2.1
1	B	442	GLY	2.1
1	B	681	VAL	2.1
1	C	947	VAL	2.1
1	C	1135	VAL	2.1
1	A	74	LEU	2.1
1	D	1323	LEU	2.1
1	D	1394	LEU	2.1
1	A	85	ALA	2.1
1	A	188	ALA	2.1
1	A	206	ALA	2.1
1	C	828	ALA	2.1
1	C	1038	ALA	2.1
1	D	1544	ALA	2.1
1	D	1251	PHE	2.0
1	C	1073	SER	2.0
1	D	1534	ILE	2.0
1	B	688	TYR	2.0
1	C	1043	TYR	2.0
1	D	1460	TYR	2.0
1	B	521	LEU	2.0
1	D	1348	ALA	2.0
1	D	1412	GLU	2.0
1	D	1363	SER	2.0
1	A	31	ILE	2.0
1	D	1549	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	962	GLY	2.0
1	D	1354	PRO	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](#)

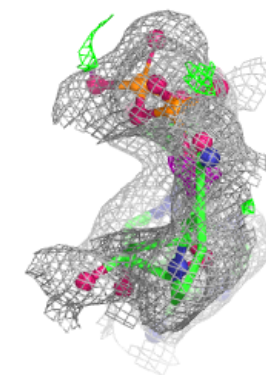
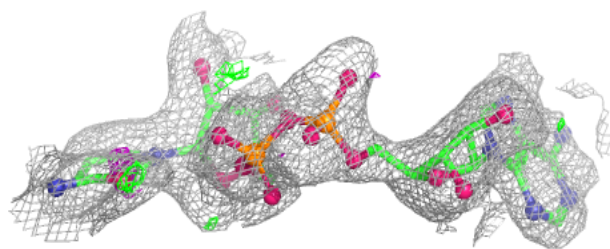
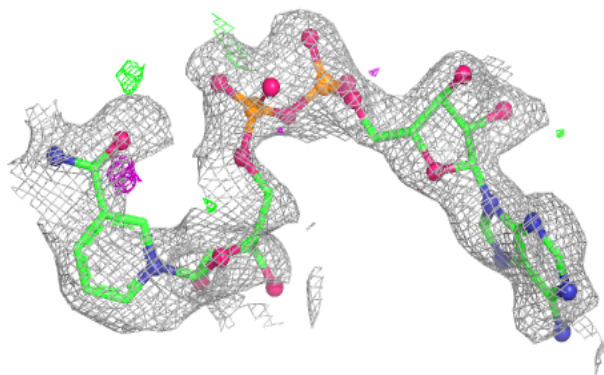
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	C	1195	5/5	0.71	0.25	16,36,53,92	0
4	K	C	1197	1/1	0.83	0.14	60,60,60,60	0
2	PO4	D	1595	5/5	0.88	0.17	28,51,72,87	0
3	NAD	D	1596	44/44	0.89	0.11	14,45,64,81	0
3	NAD	A	396	44/44	0.89	0.11	26,49,70,80	0
4	K	B	797	1/1	0.90	0.10	67,67,67,67	0
3	NAD	B	796	44/44	0.90	0.12	22,49,65,96	0
3	NAD	C	1196	44/44	0.91	0.12	18,43,76,109	0
2	PO4	B	795	5/5	0.96	0.11	32,37,61,62	0
2	PO4	A	395	5/5	0.97	0.10	22,27,48,78	0

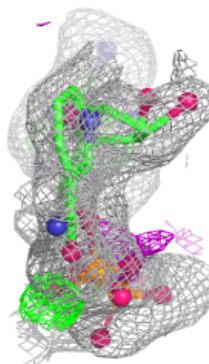
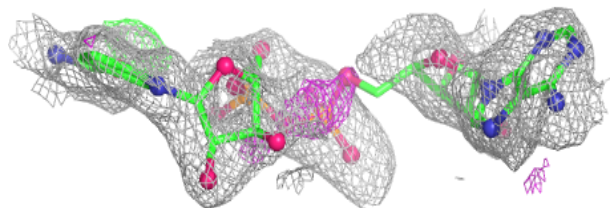
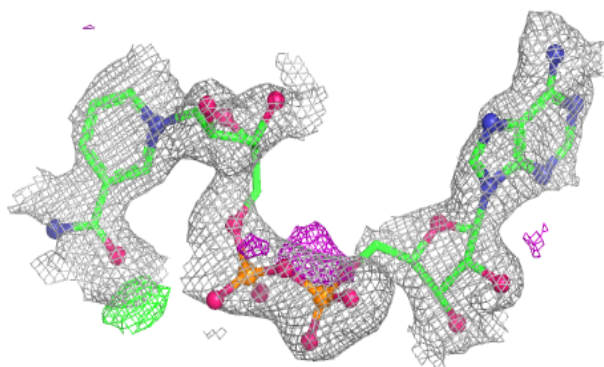
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 1596:

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

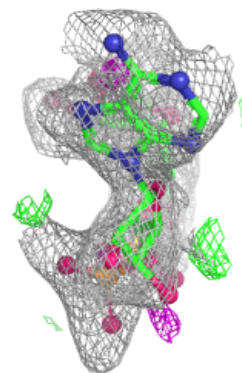
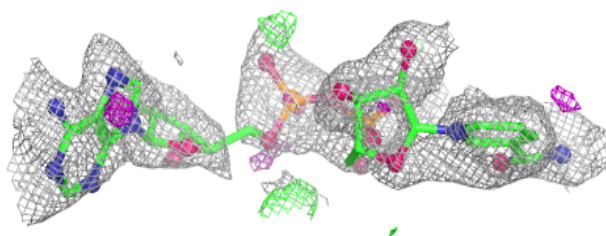
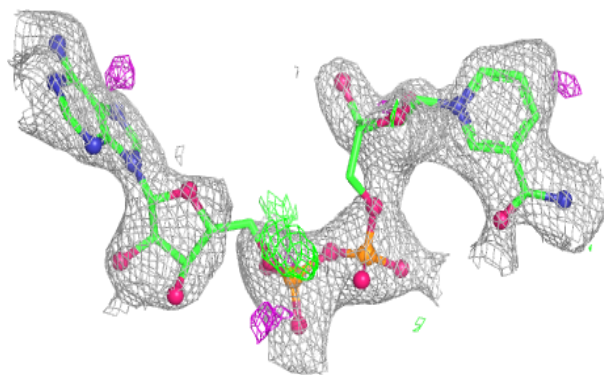
**Electron density around NAD A 396:**

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

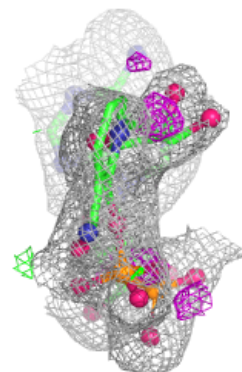
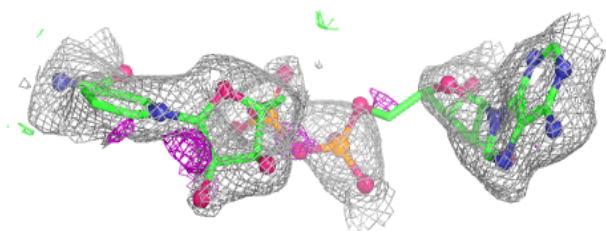
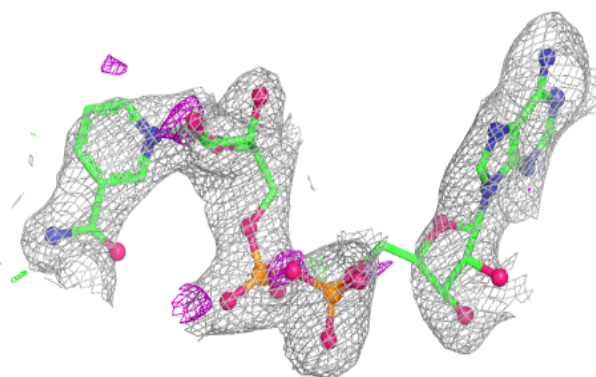


Electron density around NAD B 796:

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

**Electron density around NAD C 1196:**

$2mF_o-DF_c$ (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.