



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:27 am BST

PDB ID : 1U1I
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

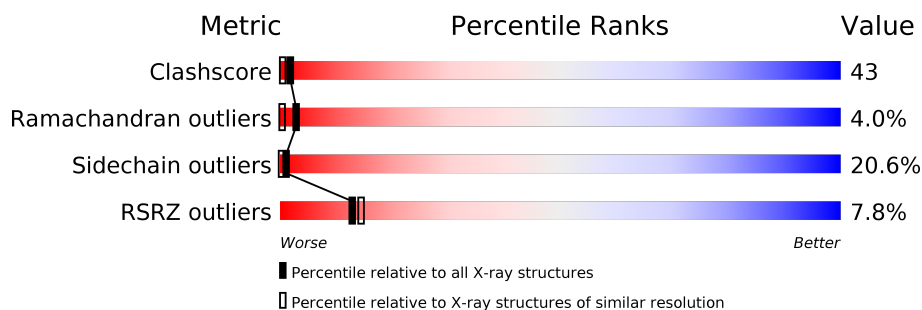
1 Overall quality at a glance

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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on 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	<div> <div>6%</div> <div>32%</div> <div>51%</div> <div>16%</div> <div>.</div> </div>
1	B	392	<div> <div>11%</div> <div>31%</div> <div>57%</div> <div>12%</div> </div>
1	C	392	<div> <div>6%</div> <div>34%</div> <div>54%</div> <div>11%</div> <div>.</div> </div>
1	D	392	<div> <div>8%</div> <div>28%</div> <div>56%</div> <div>15%</div> <div>.</div> </div>

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 (three-letter code: PO4) (formula: O₄P).



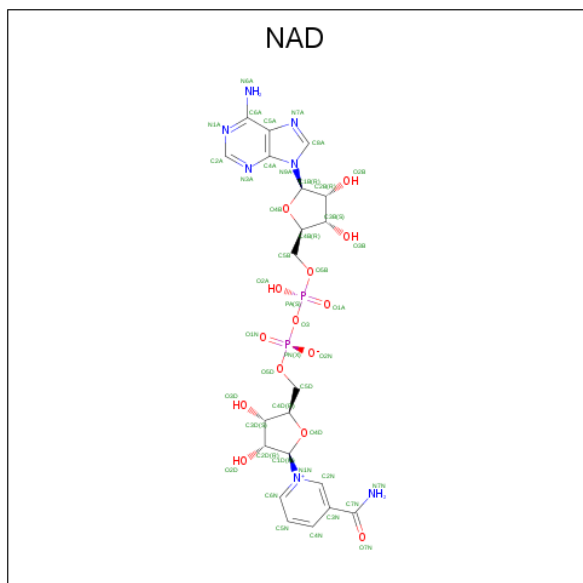
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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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 (three-letter code: 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 (three-letter code: 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		

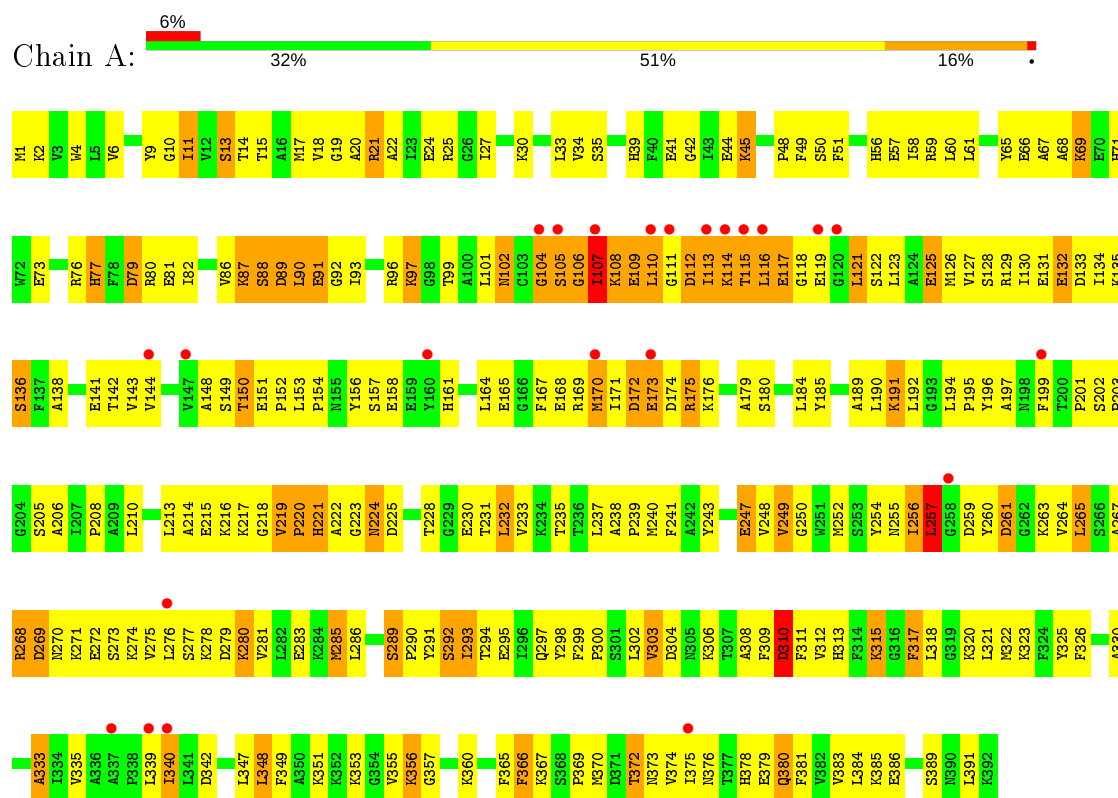
- Molecule 5 is water.

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

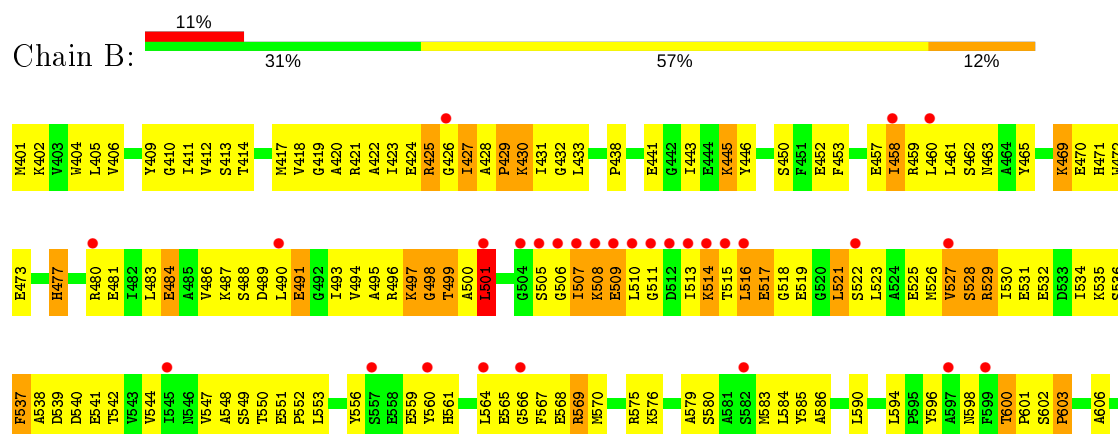
3 Residue-property plots

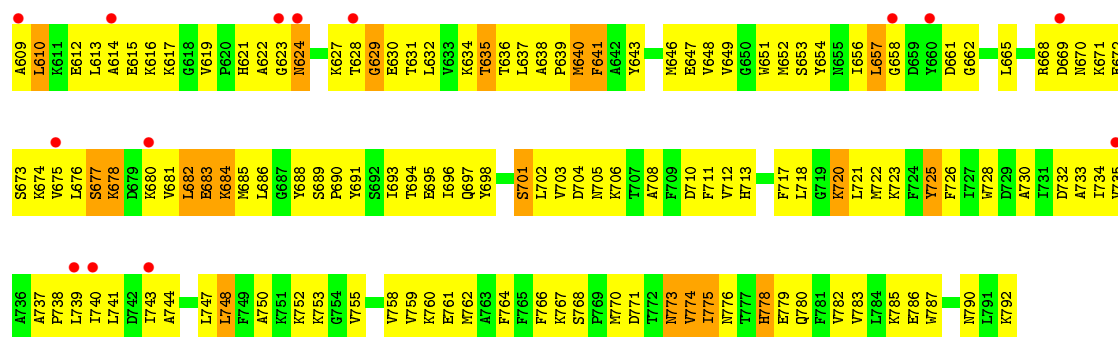
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: myo-inositol-1-phosphate synthase

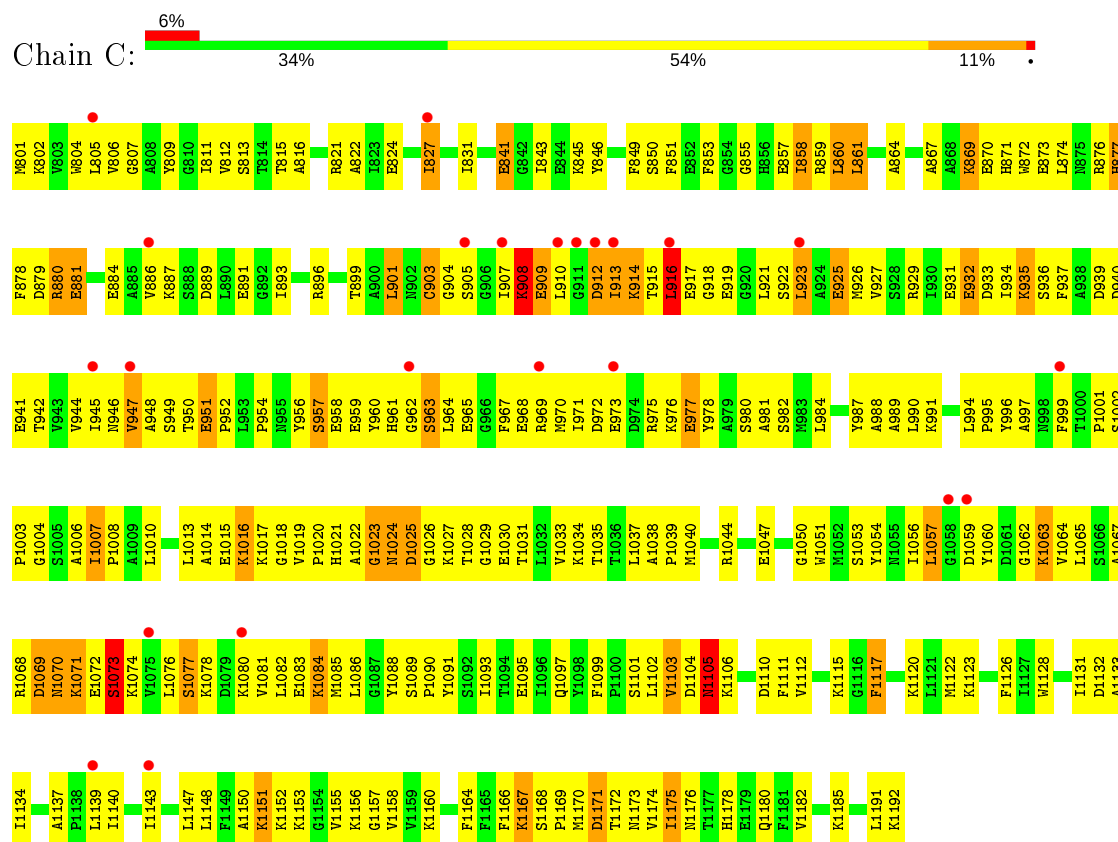


• Molecule 1: myo-inositol-1-phosphate synthase

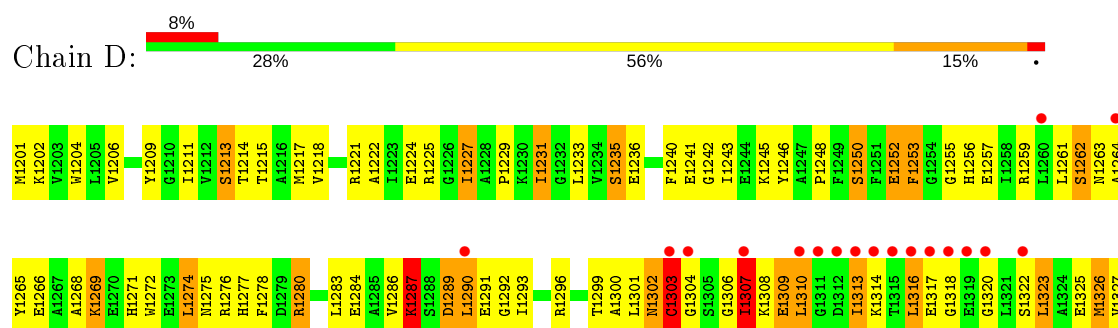


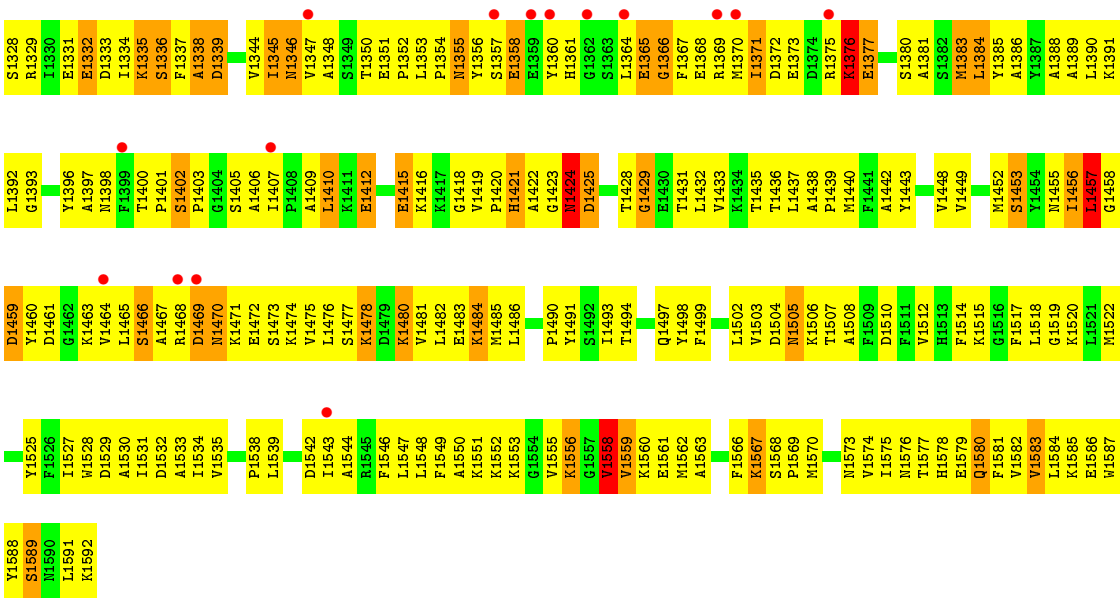


• Molecule 1: myo-inositol-1-phosphate synthase



• 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 37.65 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.60-1.90) 73.2 (37.65-1.90)	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)	0.36 , 248.3	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, PO4, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/3155	0.83	3/4257 (0.1%)
1	B	0.31	0/3155	0.82	1/4257 (0.0%)
1	C	0.31	0/3155	0.84	2/4257 (0.0%)
1	D	0.30	0/3155	0.82	0/4257
All	All	0.31	0/12620	0.83	6/17028 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ALA	C-N-CA	7.75	138.58	122.30
1	C	1023	GLY	C-N-CA	7.32	139.99	121.70
1	A	257	LEU	CA-CB-CG	6.04	129.20	115.30
1	B	643	TYR	CB-CG-CD2	5.81	124.49	121.00
1	A	310	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	C	1128	TRP	C-N-CA	5.06	134.35	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3084	0	3084	264	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3084	0	3081	281	0
1	C	3084	0	3081	270	0
1	D	3084	0	3081	300	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	6	0
5	D	232	0	0	9	0
All	All	13553	0	12430	1067	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 43.

All (1067) 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: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: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:B:776:ASN:HB3	1:B:779:GLU:HB2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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:1476:LEU:HD22	1:D:1480:LYS:HZ2	1.50	0.77
1:D:1532:ASP:HB3	3:D:1596:NAD:H72N	1.48	0.77
1:C:1069:ASP:O	1:C:1072:GLU:HB3	1.85	0.77
1:C:904:GLY:O	1:C:907:ILE:HG13	1.84	0.77
1:C:1031:THR:O	1:C:1035:THR:HG23	1.85	0.77
1:D:1421:HIS:O	1:D:1558:VAL:HA	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:490:LEU:HA	1:B:493:ILE:HG13	1.69	0.74
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1117:PHE:HA	1:D:1231:ILE:O	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:A:240:MET:HB2	1:B:636:THR:HG21	1.72	0.71
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:D:1474:LYS:HE2	1:D:1567:LYS:HZ1	1.54	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:417:MET:HE1	1:B:453:PHE:HB3	1.74	0.69
1:B:497:LYS:HD2	1:B:497:LYS:H	1.56	0.69
1:D:1435:THR:HA	1:D:1485:MET:HE1	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1006:ALA:HA	1:C:1170:MET:HE3	1.77	0.67
1:A:60:LEU:HB2	1:A:97:LYS:HZ1	1.59	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:D:1217:MET:HE3	1:D:1253:PHE:HB2	1.76	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:D:1476:LEU:HD22	1:D:1480:LYS:NZ	2.11	0.66
1:B:421:ARG:O	1:B:425:ARG:HG3	1.95	0.66
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:915:THR:O	1:C:919:GLU:HG3	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:1176:ASN:O	1:C:1180:GLN:HG3	1.97	0.65
1:C:960:TYR:HB3	1:C:970:MET:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:O	1:A:158:GLU:HG3	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:D:1559:VAL:HB	1:D:1562:MET:HE2	1.81	0.62
1:A:65:TYR:CE1	1:A:87:LYS:HB2	2.35	0.62
1:C:801:MET:HE3	1:C:1148:LEU:HD22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1476:LEU:HB3	1:D:1480:LYS:HZ2	1.65	0.62
1:D:1456:ILE:HD12	1:D:1502:LEU:HD11	1.81	0.62
1:B:741:LEU:O	1:B:744:ALA:HB3	1.99	0.61
1:A:378:HIS:ND1	1:B:778:HIS:HB2	2.15	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:1064:VAL:HG13	1:C:1070:ASN:ND2	2.16	0.60
1:C:804:TRP:CE2	1:C:855:GLY:HA2	2.36	0.60
1:A:257:LEU:HB3	1:A:306:LYS:HA	1.83	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: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:A:58:ILE:O	1:A:110:LEU:HD22	2.02	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:233:VAL:HG22	1:B:640:MET:CE	2.33	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:A:123:LEU:O	1:A:127:VAL:HG23	2.03	0.58
1:A:82:ILE:O	1:A:86:VAL:HG23	2.03	0.58
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:237:LEU:HB2	5:A:1803:HOH:O	2.03	0.58
1:A:220:PRO:HA	1:A:357:GLY:O	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1280:ARG:O	1:D:1283:LEU:HB3	2.03	0.57
1:D:1246:TYR:CE1	1:D:1553:LYS:HE2	2.39	0.57
1:A:381:PHE:CE1	1:A:385:LYS:HE2	2.39	0.57
1:A:65:TYR:OH	1:A:69:LYS:HD3	2.05	0.57
1:B:564:LEU:O	1:B:568:GLU:HB2	2.05	0.57
1:A:235:THR:HG22	1:A:281:VAL:HG11	1.86	0.57
1:A:77:HIS:H	1:A:77:HIS:CD2	2.23	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:A:9:TYR:CE2	1:A:61:LEU:HB2	2.40	0.56
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:D:1354:PRO:CB	1:D:1403:PRO:HG3	2.35	0.56
1:A:10:GLY:HA3	5:A:1604:HOH:O	2.05	0.56
1:B:675:VAL:HG13	1:B:694:THR:CG2	2.36	0.56
1:C:1033:VAL:HG22	1:D:1440:MET:HE1	1.88	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:O	1:D:1307:ILE:HD13	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:B:570:MET:HE3	1:B:579:ALA:HB2	1.88	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:167:PHE:O	1:A:170:MET:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:HG3	1:A:88:SER:N	2.21	0.55
1:C:861:LEU:HD22	1:C:867:ALA:HA	1.88	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: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:H	1:D:1531:ILE:HD12	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
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:B:432:GLY:O	1:B:738:PRO:HB2	2.06	0.55
1:C:1153:LYS:HE3	1:C:1191:LEU:O	2.06	0.55
1:C:813:SER:O	1:C:816:ALA:HB3	2.06	0.55
1:A:248:VAL:O	1:A:290:PRO:HB3	2.06	0.54
1:D:1277:HIS:CD2	1:D:1277:HIS:H	2.23	0.54
1:A:268:ARG:HH11	1:A:268:ARG:HG3	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: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:B:513:ILE:O	1:B:514:LYS:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1070:ASN:O	1:C:1073:SER:HB2	2.08	0.54
1:C:932:GLU:HA	1:C:935:LYS:HD2	1.89	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:1153:LYS:CB	1:C:1191:LEU:HD22	2.37	0.54
1:C:853:PHE:HB2	1:C:893:ILE:HD13	1.89	0.54
1:C:1015:GLU:HG2	1:C:1157:GLY:HA2	1.89	0.54
1:C:805:LEU:HD13	1:C:813:SER:OG	2.08	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
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:D:1514:PHE:CE2	1:D:1522:MET:HE3	2.43	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:A:233:VAL:HG22	1:B:640:MET:HE3	1.91	0.53
1:B:411:ILE:HG12	1:B:733:ALA:CB	2.39	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:HG2	1:B:570:MET:O	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: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:1120:LYS:CB	1:D:1534:ILE:HD13	2.38	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:680:LYS:HZ3	1:B:683:GLU:HB2	1.74	0.52
1:C:809:TYR:HB2	1:C:857:GLU:OE1	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
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: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:A:60:LEU:HD13	1:A:97:LYS:CE	2.40	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: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:A:228:THR:HG22	1:A:339:LEU:CD1	2.40	0.52
1:A:9:TYR:O	1:A:71:HIS:HE1	1.93	0.52
1:C:1139:LEU:O	1:C:1143:ILE:HG13	2.10	0.52
1:A:56:HIS:CE1	1:A:130:ILE:HG23	2.45	0.52
1:A:376:ASN:HB3	1:A:379:GLU:OE2	2.10	0.52
1:B:567:PHE:O	1:B:570:MET:HB3	2.09	0.52
1:A:297:GLN:HG3	1:C:1095:GLU:OE1	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1357:SER:CB	1:D:1360:TYR:HB2	2.41	0.51
1:C:1040:MET:HE1	1:D:1433:VAL:HA	1.92	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:1057:LEU:HD13	1:C:1062:GLY:CA	2.41	0.51
1:C:853:PHE:HB2	1:C:893:ILE:CD1	2.41	0.51
1:C:913:ILE:O	1:C:913:ILE:HG23	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:D:1217:MET:CE	1:D:1293:ILE:HG21	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: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:ND2	1:D:1470:ASN:H	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:D:1422:ALA:HB2	1:D:1559:VAL:H	1.76	0.51
1:C:1178:HIS:ND1	1:D:1578:HIS:HB3	2.26	0.51
1:D:1576:ASN:O	1:D:1580:GLN:HG3	2.11	0.51
1:A:173:GLU:OE2	1:A:173:GLU:HA	2.11	0.51
1:A:230:GLU:CD	1:A:255:ASN:HD21	2.15	0.51
1:C:1006:ALA:HA	1:C:1170:MET:CE	2.41	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:H	1:B:778:HIS:CD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:176:LYS:HA	1:A:179:ALA:HB3	1.93	0.50
1:A:99:THR:HG22	1:A:185:TYR:CZ	2.47	0.50
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:1217:MET:HE2	1:D:1253:PHE:CD1	2.47	0.50
1:D:1263:ASN:OD1	1:D:1291:GLU:OE1	2.30	0.50
1:A:230:GLU:OE1	1:A:310:ASP:OD2	2.29	0.50
1:A:97:LYS:HG2	1:A:115:THR:CB	2.38	0.50
1:B:422:ALA:HB1	1:B:428:ALA:HB2	1.94	0.50
1:B:635:THR:HA	1:B:685:MET:HE1	1.93	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: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:C:880:ARG:O	1:C:884:GLU:OE1	2.30	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:B:401:MET:CE	1:B:748:LEU:HD22	2.42	0.50
1:A:21:ARG:O	1:A:25:ARG:HG3	2.11	0.50
1:C:965:GLU:O	1:C:965:GLU:HG2	2.10	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: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:1211:ILE:HG12	1:D:1533:ALA:CB	2.42	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:1117:PHE:CG	1:D:1538:PRO:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1328:SER:O	1:D:1332:GLU:OE1	2.30	0.49
1:A:105:SER:H	1:A:269:ASP:CG	2.15	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:D:1474:LYS:HE2	1:D:1567:LYS:NZ	2.25	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
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:1072:GLU:O	1:C:1076:LEU:HG	2.12	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: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: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:114:LYS:HG2	1:A:119:GLU:CA	2.40	0.49
1:A:96:ARG:CD	1:A:133:ASP:HB3	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: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:C:805:LEU:O	1:C:855:GLY:HA3	2.11	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:249:VAL:HG21	1:A:321:LEU:HD21	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:507:ILE:HD13	1:B:508:LYS:N	2.28	0.48
1:B:459:ARG:HB2	1:B:510:LEU:HD11	1.94	0.48
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: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:A:141:GLU:HB3	1:A:348:LEU:HD21	1.96	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:196:TYR:CE1	1:A:205:SER:HB3	2.49	0.48
1:A:33:LEU:HD13	1:A:49:PHE:HE1	1.77	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:B:515:THR:HG22	1:B:515:THR:O	2.13	0.48
1:D:1346:ASN:HD21	1:D:1400:THR:HG23	1.78	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: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:C:801:MET:CE	1:C:1148:LEU:HD22	2.44	0.47
1:D:1474:LYS:HE3	3:D:1596:NAD:C6N	2.43	0.47
1:A:221:HIS:CD2	1:A:221:HIS:H	2.31	0.47
1:A:90:LEU:HA	1:A:93:ILE:CD1	2.37	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:164:LEU:HD13	1:A:213:LEU:HB2	1.96	0.47
1:A:61:LEU:HD11	5:A:1999:HOH:O	2.14	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:1040:MET:CE	1:D:1432:LEU:HG	2.45	0.47
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:HG23	1:D:1307:ILE:O	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: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:1455:ASN:HD22	1:D:1506:LYS:NZ	2.12	0.47
1:D:1453:SER:HB3	1:D:1494:THR:HG23	1.97	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: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:C:1152:LYS:HE2	5:C:1801:HOH:O	2.13	0.47
1:D:1304:GLY:HA3	1:D:1307:ILE:HG21	1.96	0.47
1:A:260:TYR:CA	1:A:263:LYS:HG3	2.42	0.47
1:C:1172:THR:OG1	1:C:1174:VAL:HG23	2.15	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: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:411:ILE:HD11	1:B:477:HIS:NE2	2.30	0.47
1:B:553:LEU:HD13	1:B:672:GLU:HB3	1.97	0.47
1:C:1038:ALA:HB3	1:C:1085:MET:HE1	1.96	0.47
1:D:1476:LEU:CD2	1:D:1480:LYS:HZ2	2.25	0.47
1:C:1126:PHE:HB2	1:D:1525:TYR:O	2.15	0.47
1:A:114:LYS:O	1:A:115:THR:OG1	2.30	0.47
1:A:317:PHE:O	1:A:318:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:982:SER:O	1:C:1004:GLY:HA2	2.15	0.47
1:C:1040:MET:CE	1:D:1433:VAL:HA	2.45	0.47
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:D:1306:GLY:C	1:D:1464:VAL:HG13	2.35	0.47
1:C:859:ARG:NH1	1:C:861:LEU:HD11	2.30	0.46
1:D:1370:MET:HG2	1:D:1371:ILE:N	2.29	0.46
1:C:1120:LYS:HG2	1:D:1534:ILE:HD13	1.97	0.46
1:A:254:TYR:HD2	1:A:295:GLU:HB2	1.80	0.46
1:D:1345:ILE:O	1:D:1345:ILE:HG22	2.15	0.46
1:D:1452:MET:O	1:D:1510:ASP:HA	2.14	0.46
1:A:320:LYS:HD2	1:A:321:LEU:N	2.30	0.46
1:A:61:LEU:HD12	1:A:67:ALA:CB	2.42	0.46
1:B:782:VAL:O	1:B:785:LYS:HB2	2.14	0.46
1:C:1084:LYS:HG3	1:C:1084:LYS:H	1.47	0.46
1:C:932:GLU:HG2	1:C:935:LYS:NZ	2.30	0.46
1:B:701:SER:HB2	1:D:1449:VAL:HG12	1.97	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:628:THR:O	1:B:629:GLY:O	2.32	0.46
1:B:623:GLY:HA2	1:B:766:PHE:CZ	2.51	0.46
1:C:1018:GLY:HA2	1:C:1156:LYS:HB2	1.97	0.46
1:C:965:GLU:CD	1:C:969:ARG:HH21	2.18	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:1221:ARG:HE	1:D:1289:ASP:HB3	1.81	0.46
1:D:1206:VAL:HG21	1:D:1385:TYR:CG	2.49	0.46
1:C:1040:MET:HE1	1:D:1432:LEU:HG	1.98	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:1217:MET:HE3	1:D:1293:ILE:HG21	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:551:GLU:HG3	1:B:602:SER:CB	2.46	0.45
1:C:1064:VAL:O	1:C:1070:ASN:ND2	2.49	0.45
1:B:480:ARG:CD	1:C:880:ARG:HD2	2.45	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:1051:TRP:CD2	1:C:1112:VAL:HG22	2.51	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:D:1272:TRP:HE1	1:D:1278:PHE:C	2.19	0.45
1:D:1314:LYS:HD3	1:D:1318:GLY:HA2	1.98	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: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: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:OD1	1:C:1171:ASP:N	2.50	0.45
1:C:916:LEU:HD11	1:C:926:MET:HB3	1.89	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:1105:ASN:HA	1:C:1131:ILE:HD13	1.97	0.45
1:C:941:GLU:HB3	1:C:1148:LEU:HD21	1.97	0.45
1:D:1539:LEU:N	1:D:1539:LEU:HD23	2.31	0.45
1:A:243:TYR:OH	1:A:376:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:O	1:A:61:LEU:HD23	2.16	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
1:D:1269:LYS:NZ	5:D:2559:HOH:O	2.50	0.45
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:A:252:MET:HE2	1:A:309:PHE:O	2.16	0.45
1:B:417:MET:CE	1:B:453:PHE:HB3	2.45	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:B:446:TYR:O	1:B:752:LYS:NZ	2.50	0.45
1:C:1014:ALA:O	1:C:1018:GLY:N	2.50	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: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:B:427:ILE:HG23	1:B:427:ILE:O	2.16	0.45
1:C:959:GLU:OE2	1:C:959:GLU:N	2.50	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:B:539:ASP:OD2	1:B:542:THR:OG1	2.30	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:D:1472:GLU:O	1:D:1476:LEU:HG	2.17	0.44
1:D:1277:HIS:HB2	1:D:1534:ILE:CD1	2.47	0.44
1:A:110:LEU:HD13	1:A:113:ILE:HG21	1.98	0.44
1:B:647:GLU:HG3	1:B:648:VAL:N	2.32	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1400:THR:O	1:D:1425:ASP:N	2.50	0.44
1:A:214:ALA:O	1:A:218:GLY:N	2.50	0.44
1:A:285:MET:HB2	1:A:285:MET:HE2	1.87	0.44
1:A:24:GLU:OE2	1:A:51:PHE:N	2.49	0.44
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:HA	1:D:1290:LEU:HD12	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:497:LYS:HG2	1:B:516:LEU:HD23	2.00	0.44
1:B:402:LYS:HB3	1:B:542:THR:HG23	2.00	0.44
1:C:997:ALA:HB2	1:C:1147:LEU:HD11	1.98	0.44
1:C:944:VAL:HG12	1:C:996:TYR:CD1	2.52	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: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:C:807:GLY:HA2	3:C:1196:NAD:N3A	2.31	0.44
1:A:150:THR:HG22	1:A:270:ASN:HB3	1.99	0.44
1:A:22:ALA:HB2	1:A:82:ILE:HG23	1.98	0.44
1:B:723:LYS:NZ	1:D:1529:ASP:OD2	2.50	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:C:881:GLU:HG3	1:C:881:GLU:H	1.45	0.44
1:C:802:LYS:HD2	1:C:939:ASP:CG	2.38	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:1418:GLY:C	1:D:1556:LYS:HB2	2.37	0.44
1:D:1428:THR:CG2	3:D:1596:NAD:H4N	2.48	0.44
1:D:1406:ALA:HA	1:D:1570:MET:HE1	2.00	0.44
1:A:144:VAL:HG21	1:A:189:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:383:VAL:O	1:A:386:GLU:HB2	2.18	0.43
1:B:569:ARG:HG2	1:B:570:MET:N	2.32	0.43
1:B:621:HIS:O	1:B:622:ALA:HB2	2.17	0.43
1:B:680:LYS:NZ	1:B:684:LYS:HB2	2.32	0.43
1:C:815:THR:HB	1:C:1137:ALA:HB2	2.00	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:C:1132:ASP:N	1:C:1132:ASP:OD1	2.50	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:D:1567:LYS:C	1:D:1569:PRO:HD3	2.39	0.43
1:A:260:TYR:O	1:A:263:LYS:HB2	2.19	0.43
1:A:9:TYR:CD2	1:A:57:GLU:HG3	2.53	0.43
1:B:425:ARG:NH2	1:B:489:ASP:OD1	2.51	0.43
1:C:1057:LEU:HD12	1:C:1057:LEU:N	2.33	0.43
1:C:995:PRO:HA	1:C:1019:VAL:CG1	2.47	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:1105:ASN:CA	1:C:1131:ILE:HD13	2.48	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: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:A:241:PHE:CZ	1:A:312:VAL:HG11	2.53	0.43
1:A:68:ALA:HA	5:A:1919:HOH:O	2.18	0.43
1:B:638:ALA:HB3	1:B:639:PRO:HD3	2.01	0.43
1:C:1185:LYS:NZ	5:C:2141:HOH:O	2.52	0.43
1:D:1410:LEU:HA	1:D:1410:LEU:HD22	1.83	0.43
1:D:1481:VAL:HG12	1:D:1482:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1345:ILE:CD1	1:D:1544:ALA:HB2	2.49	0.43
1:D:1549:PHE:CZ	1:D:1591:LEU:HB2	2.54	0.43
1:B:688:TYR:C	1:B:690:PRO:HD3	2.39	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
1:D:1436:THR:HG22	1:D:1436:THR:O	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:1068:ARG:O	1:C:1072:GLU:HB2	2.19	0.43
1:C:1020:PRO:HB3	1:C:1155:VAL:HG12	2.01	0.43
1:C:841:GLU:HG3	1:C:841:GLU:H	1.59	0.43
1:A:233:VAL:HG22	1:B:640:MET:HE1	2.00	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: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:D:1243:ILE:HD12	1:D:1588:TYR:HE1	1.84	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:1068:ARG:HG2	1:C:1068:ARG:O	2.19	0.43
1:C:913:ILE:O	1:C:915:THR:N	2.50	0.43
1:D:1429:GLY:HA3	1:D:1528:TRP:CZ2	2.54	0.43
1:A:106:GLY:C	1:A:264:VAL:HG22	2.40	0.42
1:A:369:PRO:HB2	1:A:372:THR:HG22	2.00	0.42
1:A:89:ASP:OD2	1:A:89:ASP:N	2.50	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: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:1023:GLY:HA2	1:C:1166:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1030:GLU:HB3	2:C:1195:PO4:O3	2.19	0.42
1:C:901:LEU:H	1:C:981:ALA:HB2	1.84	0.42
1:A:13:SER:OG	1:A:14:THR:N	2.52	0.42
1:A:257:LEU:HD21	1:A:261:ASP:HB2	2.00	0.42
1:A:73:GLU:HG3	1:A:73:GLU:O	2.19	0.42
1:B:411:ILE:HG13	1:B:477:HIS:HE2	1.84	0.42
1:C:1033:VAL:CG2	1:D:1440:MET:HE1	2.50	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: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: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: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:758:VAL:CG1	1:B:770:MET:HB2	2.48	0.42
1:B:500:ALA:HB2	3:B:796:NAD:N6A	2.34	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: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: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:1139:LEU:HD23	1:C:1139:LEU:N	2.34	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: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:412:VAL:HG11	1:B:547:VAL:HG21	2.02	0.42
1:B:406:VAL:HG21	1:B:585:TYR:CD1	2.54	0.42
1:C:1131:ILE:CG2	1:C:1134:ILE:HD13	2.50	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:372:THR:HG23	1:A:373:ASN:N	2.34	0.42
1:A:39:HIS:CD2	1:A:385:LYS:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:870:GLU:OE2	1:C:1060:TYR:OH	2.30	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:B:722:MET:HB2	1:B:722:MET:HE3	1.90	0.41
1:B:774:VAL:C	1:B:775:ILE:HD13	2.41	0.41
1:C:1024:ASN:O	1:C:1168:SER:HB2	2.20	0.41
1:C:945:ILE:HG12	1:C:997:ALA:HB3	2.02	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:615:GLU:OE1	1:B:615:GLU:HA	2.20	0.41
1:B:739:LEU:HD23	1:B:739:LEU:N	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:1559:VAL:HG21	1:D:1562:MET:HE1	2.02	0.41
1:A:378:HIS:HB3	5:A:1787:HOH:O	2.19	0.41
1:A:90:LEU:HA	1:A:90:LEU:HD22	1.90	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:1329:ARG:CA	1:D:1332:GLU:HB2	2.49	0.41
1:B:691:TYR:OH	1:D:1498:TYR:O	2.30	0.41
1:D:1246:TYR:HD1	1:D:1549:PHE:HD2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:THR:HB	1:A:375:ILE:O	2.21	0.41
1:C:923:LEU:HA	1:C:923:LEU:HD12	1.85	0.41
1:A:116:LEU:HB3	1:A:117:GLU:H	1.57	0.41
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:HD13	1:A:340:ILE:N	2.35	0.41
1:A:57:GLU:OE2	3:A:396:NAD:O3B	2.30	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
5:A:2516:HOH:O	1:D:1280:ARG:HG2	2.21	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:142:THR:O	1:A:143:VAL:HG13	2.20	0.41
1:A:15:THR:O	1:A:15:THR:HG22	2.20	0.41
1:B:743:ILE:HA	1:B:762:MET:HE1	2.02	0.41
1:C:1089:SER:HA	1:C:1090:PRO:HD2	1.94	0.41
1:C:1018:GLY:HA2	1:C:1156:LYS:CB	2.51	0.41
1:C:889:ASP:OD2	1:C:889:ASP:N	2.52	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:A:142:THR:HG22	1:A:143:VAL:N	2.36	0.41
1:A:1:MET:N	1:A:50:SER:O	2.50	0.41
1:C:859:ARG:HG3	1:C:910:LEU:CD1	2.35	0.41
1:D:1377:GLU:HG3	5:D:2346:HOH:O	2.21	0.41
1:D:1455:ASN:HD22	1:D:1506:LYS:HZ3	1.68	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:A:57:GLU:OE2	3:A:396:NAD:H1B	2.20	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:1508:ALA:O	1:D:1527:ILE:HA	2.20	0.41
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:A:11:ILE:HD13	1:A:333:ALA:CB	2.47	0.40
1:A:216:LYS:HG3	1:A:216:LYS:O	2.21	0.40
1:A:239:PRO:HB3	1:A:243:TYR:CZ	2.57	0.40
1:B:428:ALA:HA	1:B:429:PRO:HD3	1.93	0.40
1:B:418:VAL:HG22	1:B:490:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:685:MET:HB2	1:B:685:MET:HE2	1.80	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:HG3	1:D:1358:GLU:H	1.59	0.40
1:B:412:VAL:HG22	1:B:733:ALA:HA	2.03	0.40
1:B:532:GLU:HG2	1:B:532:GLU:O	2.21	0.40
1:B:740:ILE:HD13	1:B:740:ILE:N	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:680:LYS:HZ3	1:B:683:GLU:CB	2.34	0.40
1:B:782:VAL:O	1:B:786:GLU:HG3	2.21	0.40
1:C:994:LEU:O	1:C:1019:VAL:HG11	2.22	0.40
1:C:815:THR:OG1	1:C:1133:ALA:HB1	2.21	0.40
1:C:1167:LYS:C	1:C:1169:PRO:HD3	2.42	0.40
1:D:1310:LEU:O	1:D:1313:ILE:HB	2.21	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

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%)	5	1
1	B	390/392 (100%)	331 (85%)	43 (11%)	16 (4%)	3	0
1	C	390/392 (100%)	340 (87%)	37 (10%)	13 (3%)	4	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%)	3	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%)	247 (76%)	78 (24%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	325/325 (100%)	268 (82%)	57 (18%)	2	0
1	C	325/325 (100%)	265 (82%)	60 (18%)	1	0
1	D	325/325 (100%)	252 (78%)	73 (22%)	1	0
All	All	1300/1300 (100%)	1032 (79%)	268 (21%)	1	0

All (268) 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	30	LYS
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	79	ASP
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	97	LYS
1	A	102	ASN
1	A	105	SER
1	A	107	ILE
1	A	108	LYS
1	A	110	LEU
1	A	112	ASP
1	A	113	ILE
1	A	114	LYS
1	A	116	LEU
1	A	117	GLU
1	A	121	LEU
1	A	125	GLU
1	A	128	SER

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Mol	Chain	Res	Type
1	A	132	GLU
1	A	136	SER
1	A	150	THR
1	A	156	TYR
1	A	157	SER
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	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	285	MET
1	A	286	LEU
1	A	289	SER
1	A	292	SER
1	A	293	ILE
1	A	310	ASP
1	A	315	LYS
1	A	317	PHE
1	A	340	ILE
1	A	348	LEU
1	A	356	LYS
1	A	360	LYS
1	A	366	PHE
1	A	372	THR

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Mol	Chain	Res	Type
1	A	380	GLN
1	A	384	LEU
1	A	389	SER
1	B	425	ARG
1	B	427	ILE
1	B	430	LYS
1	B	431	ILE
1	B	443	ILE
1	B	445	LYS
1	B	458	ILE
1	B	469	LYS
1	B	477	HIS
1	B	481	GLU
1	B	484	GLU
1	B	488	SER
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	516	LEU
1	B	517	GLU
1	B	521	LEU
1	B	527	VAL
1	B	528	SER
1	B	529	ARG
1	B	531	GLU
1	B	537	PHE
1	B	540	ASP
1	B	541	GLU
1	B	565	GLU
1	B	569	ARG
1	B	600	THR
1	B	610	LEU
1	B	612	GLU
1	B	635	THR
1	B	640	MET
1	B	641	PHE
1	B	653	SER
1	B	657	LEU

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Mol	Chain	Res	Type
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	720	LYS
1	B	725	TYR
1	B	734	ILE
1	B	735	VAL
1	B	748	LEU
1	B	760	LYS
1	B	773	ASN
1	B	775	ILE
1	B	778	HIS
1	B	792	LYS
1	C	812	VAL
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	878	PHE
1	C	879	ASP
1	C	880	ARG
1	C	881	GLU
1	C	891	GLU
1	C	901	LEU
1	C	903	CYS
1	C	905	SER
1	C	908	LYS
1	C	912	ASP
1	C	914	LYS
1	C	916	LEU

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Mol	Chain	Res	Type
1	C	917	GLU
1	C	923	LEU
1	C	925	GLU
1	C	932	GLU
1	C	935	LYS
1	C	940	ASP
1	C	947	VAL
1	C	949	SER
1	C	951	GLU
1	C	957	SER
1	C	963	SER
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	1017	LYS
1	C	1047	GLU
1	C	1057	LEU
1	C	1059	ASP
1	C	1063	LYS
1	C	1069	ASP
1	C	1070	ASN
1	C	1071	LYS
1	C	1073	SER
1	C	1077	SER
1	C	1084	LYS
1	C	1101	SER
1	C	1105	ASN
1	C	1110	ASP
1	C	1151	LYS
1	C	1167	LYS
1	C	1171	ASP
1	C	1175	ILE
1	C	1192	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	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	1316	LEU
1	D	1322	SER
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	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	1402	SER
1	D	1410	LEU
1	D	1412	GLU
1	D	1415	GLU
1	D	1416	LYS
1	D	1421	HIS
1	D	1424	ASN

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Mol	Chain	Res	Type
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	1477	SER
1	D	1478	LYS
1	D	1480	LYS
1	D	1483	GLU
1	D	1484	LYS
1	D	1486	LEU
1	D	1497	GLN
1	D	1499	PHE
1	D	1505	ASN
1	D	1512	VAL
1	D	1535	VAL
1	D	1551	LYS
1	D	1556	LYS
1	D	1558	VAL
1	D	1560	LYS
1	D	1567	LYS
1	D	1568	SER
1	D	1580	GLN
1	D	1589	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	77	HIS
1	A	102	ASN
1	A	161	HIS
1	B	624	ASN
1	B	697	GLN
1	B	778	HIS
1	C	839	HIS
1	C	877	HIS
1	C	1021	HIS
1	C	1173	ASN
1	D	1271	HIS
1	D	1277	HIS

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Mol	Chain	Res	Type
1	D	1302	ASN
1	D	1346	ASN
1	D	1361	HIS
1	D	1398	ASN
1	D	1424	ASN
1	D	1455	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	D	1596	-	42,48,48	1.45	5 (11%)	50,73,73	1.50	9 (18%)
2	PO4	D	1595	-	4,4,4	0.89	0	6,6,6	0.49	0
2	PO4	B	795	-	4,4,4	0.89	0	6,6,6	0.48	0
3	NAD	B	796	4	42,48,48	1.42	5 (11%)	50,73,73	1.37	7 (14%)
3	NAD	C	1196	4	42,48,48	1.44	5 (11%)	50,73,73	1.45	8 (16%)
2	PO4	A	395	-	4,4,4	0.84	0	6,6,6	0.47	0
3	NAD	A	396	-	42,48,48	2.13	8 (19%)	50,73,73	1.52	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	C	1195	-	4,4,4	0.91	0	6,6,6	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	D	1596	-	-	1/26/62/62	0/5/5/5
3	NAD	B	796	4	-	2/26/62/62	0/5/5/5
3	NAD	C	1196	4	-	7/26/62/62	0/5/5/5
3	NAD	A	396	-	-	9/26/62/62	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	396	NAD	C3N-C7N	-8.69	1.37	1.50
3	D	1596	NAD	C2N-N1N	6.18	1.42	1.35
3	A	396	NAD	C2N-N1N	6.15	1.42	1.35
3	C	1196	NAD	C2N-N1N	5.88	1.42	1.35
3	B	796	NAD	C2N-N1N	5.87	1.42	1.35
3	A	396	NAD	C2N-C3N	5.16	1.47	1.39
3	C	1196	NAD	O4B-C1B	-3.27	1.36	1.41
3	B	796	NAD	O4B-C1B	-3.05	1.36	1.41
3	D	1596	NAD	O4B-C1B	-2.88	1.37	1.41
3	A	396	NAD	O4B-C1B	-2.84	1.37	1.41
3	A	396	NAD	C2D-C1D	-2.68	1.49	1.53
3	D	1596	NAD	C2A-N1A	2.58	1.38	1.33
3	C	1196	NAD	C2A-N1A	2.56	1.38	1.33
3	A	396	NAD	C2A-N1A	2.54	1.38	1.33
3	B	796	NAD	C2A-N1A	2.51	1.38	1.33
3	A	396	NAD	C7N-N7N	2.50	1.37	1.33
3	A	396	NAD	C6N-N1N	2.46	1.41	1.35
3	B	796	NAD	C6N-N1N	2.35	1.41	1.35
3	C	1196	NAD	C6N-N1N	2.33	1.41	1.35
3	D	1596	NAD	C6N-N1N	2.29	1.41	1.35
3	C	1196	NAD	C7N-N7N	2.09	1.37	1.33
3	D	1596	NAD	C7N-N7N	2.07	1.36	1.33
3	B	796	NAD	C7N-N7N	2.06	1.36	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1596	NAD	O4B-C1B-C2B	-4.59	100.22	106.93
3	D	1596	NAD	PN-O3-PA	-4.45	117.56	132.83
3	A	396	NAD	PN-O3-PA	-4.34	117.92	132.83
3	B	796	NAD	O4B-C1B-C2B	-4.18	100.82	106.93
3	C	1196	NAD	O7N-C7N-C3N	-3.91	114.95	119.63
3	B	796	NAD	O7N-C7N-C3N	-3.87	115.00	119.63
3	C	1196	NAD	O4B-C1B-C2B	-3.52	101.78	106.93
3	A	396	NAD	O4B-C1B-C2B	-3.38	101.99	106.93
3	A	396	NAD	C5N-C4N-C3N	3.31	124.26	120.34
3	A	396	NAD	C5A-C6A-N6A	3.19	125.20	120.35
3	C	1196	NAD	C3N-C2N-N1N	-2.99	117.50	120.43
3	C	1196	NAD	PN-O3-PA	-2.98	122.59	132.83
3	D	1596	NAD	O4D-C4D-C5D	2.94	119.03	109.37
3	B	796	NAD	C3N-C2N-N1N	-2.91	117.58	120.43
3	C	1196	NAD	C5A-C6A-N6A	2.89	124.75	120.35
3	A	396	NAD	C3N-C7N-N7N	-2.87	114.30	117.75
3	C	1196	NAD	C2B-C3B-C4B	-2.67	97.46	102.64
3	D	1596	NAD	C5A-C6A-N6A	2.61	124.32	120.35
3	C	1196	NAD	C2N-C3N-C4N	2.59	121.19	118.26
3	B	796	NAD	C2N-C3N-C4N	2.58	121.18	118.26
3	B	796	NAD	C5A-C6A-N6A	2.57	124.26	120.35
3	A	396	NAD	O4D-C4D-C5D	2.54	117.72	109.37
3	D	1596	NAD	O7N-C7N-C3N	-2.39	116.77	119.63
3	D	1596	NAD	C2B-C3B-C4B	-2.35	98.07	102.64
3	D	1596	NAD	C4A-C5A-N7A	2.32	111.82	109.40
3	A	396	NAD	C2B-C3B-C4B	-2.25	98.26	102.64
3	C	1196	NAD	C4A-C5A-N7A	2.24	111.73	109.40
3	B	796	NAD	C4A-C5A-N7A	2.23	111.72	109.40
3	D	1596	NAD	O5B-C5B-C4B	-2.22	101.34	108.99
3	A	396	NAD	O5B-C5B-C4B	-2.17	101.53	108.99
3	A	396	NAD	C6N-N1N-C2N	-2.16	120.00	121.97
3	D	1596	NAD	C6N-N1N-C2N	-2.07	120.08	121.97
3	B	796	NAD	PA-O5B-C5B	-2.00	109.94	121.68

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1196	NAD	C5B-O5B-PA-O1A
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

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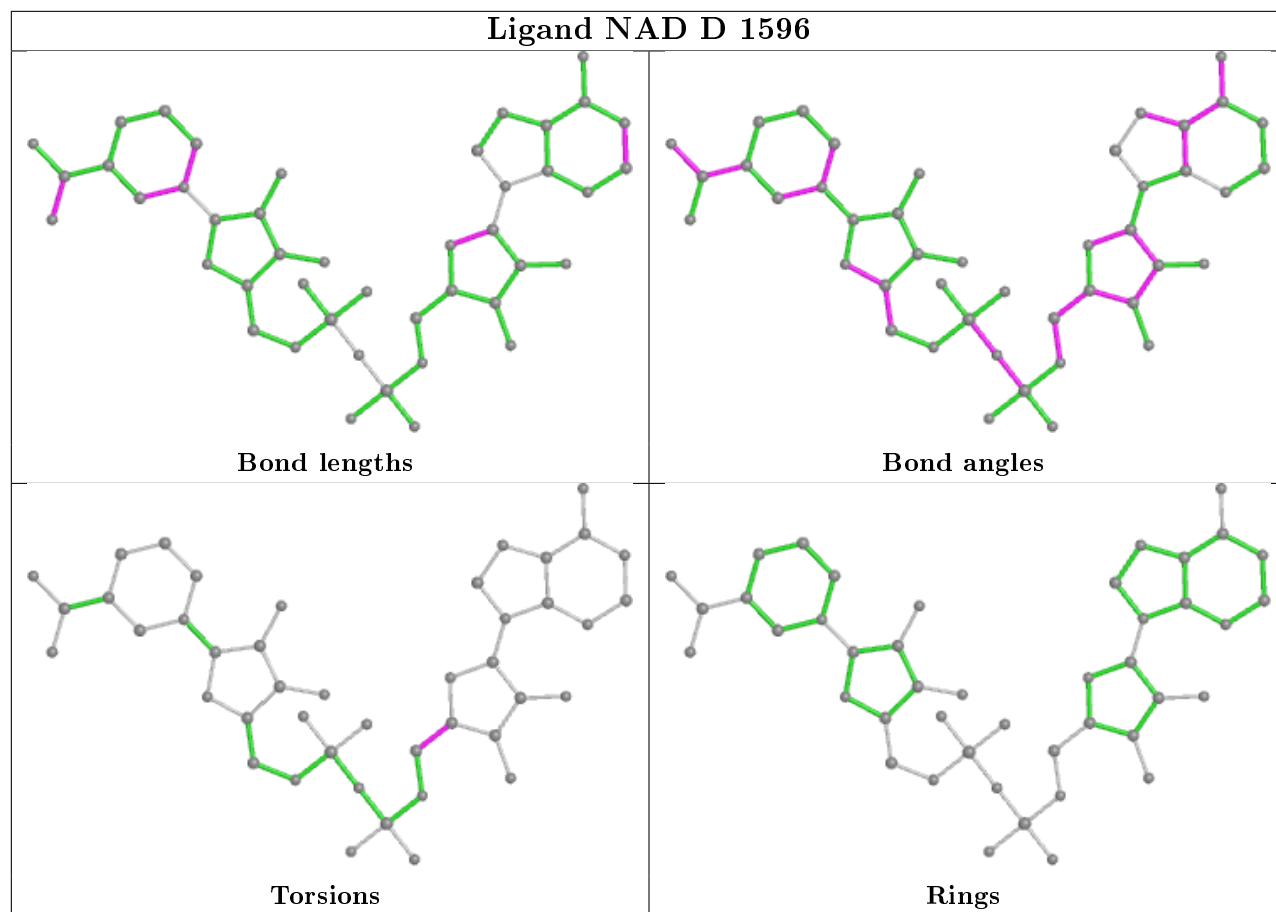
Mol	Chain	Res	Type	Atoms
3	C	1196	NAD	O4B-C4B-C5B-O5B
3	A	396	NAD	O4B-C4B-C5B-O5B
3	A	396	NAD	C3B-C4B-C5B-O5B
3	C	1196	NAD	C3B-C4B-C5B-O5B
3	A	396	NAD	O4D-C4D-C5D-O5D
3	C	1196	NAD	C5B-O5B-PA-O3
3	C	1196	NAD	C5B-O5B-PA-O2A
3	B	796	NAD	PA-O3-PN-O2N
3	D	1596	NAD	O4B-C4B-C5B-O5B
3	A	396	NAD	C5B-O5B-PA-O3
3	C	1196	NAD	PA-O3-PN-O1N
3	C	1196	NAD	PA-O3-PN-O2N
3	A	396	NAD	C5B-O5B-PA-O2A
3	B	796	NAD	O4B-C4B-C5B-O5B

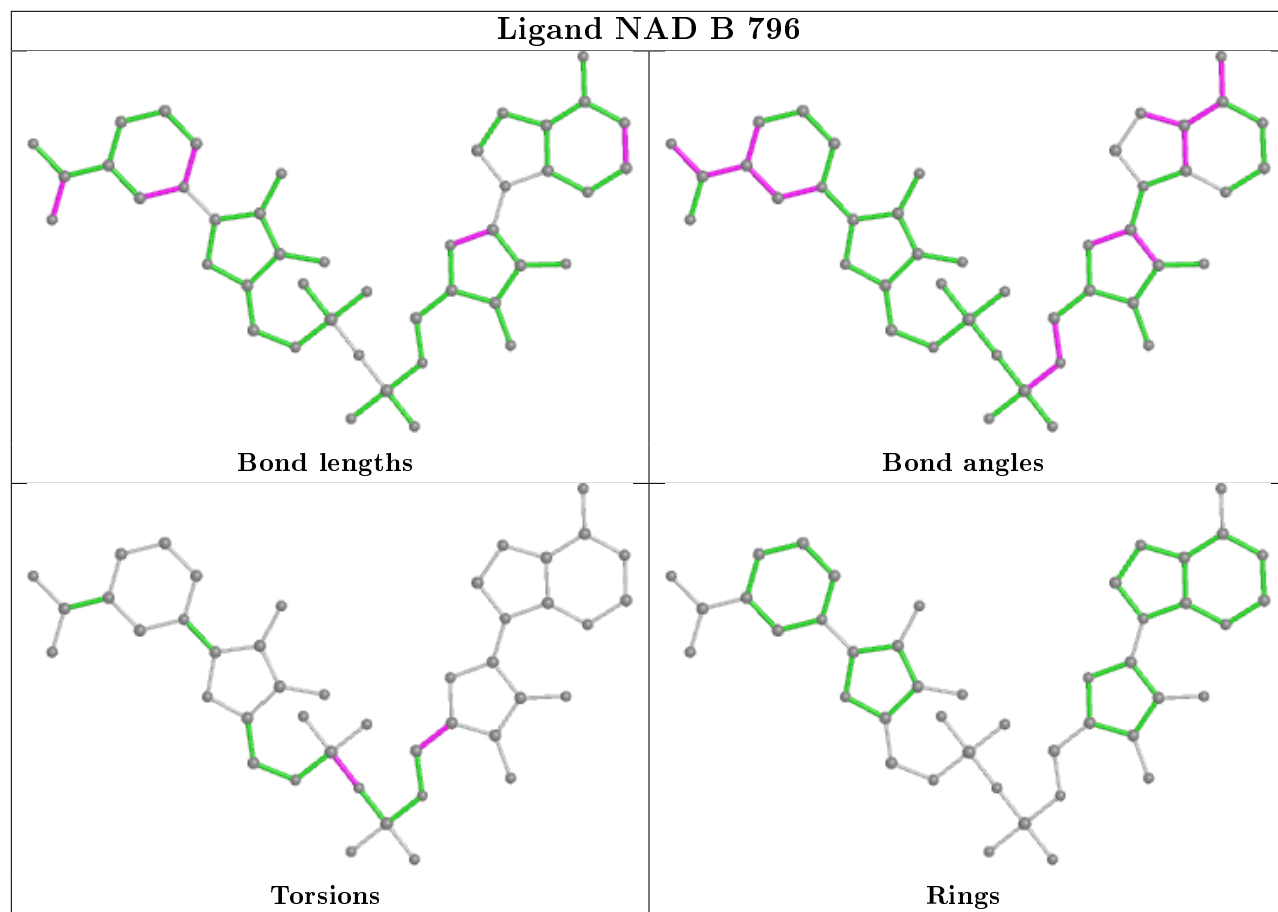
There are no ring outliers.

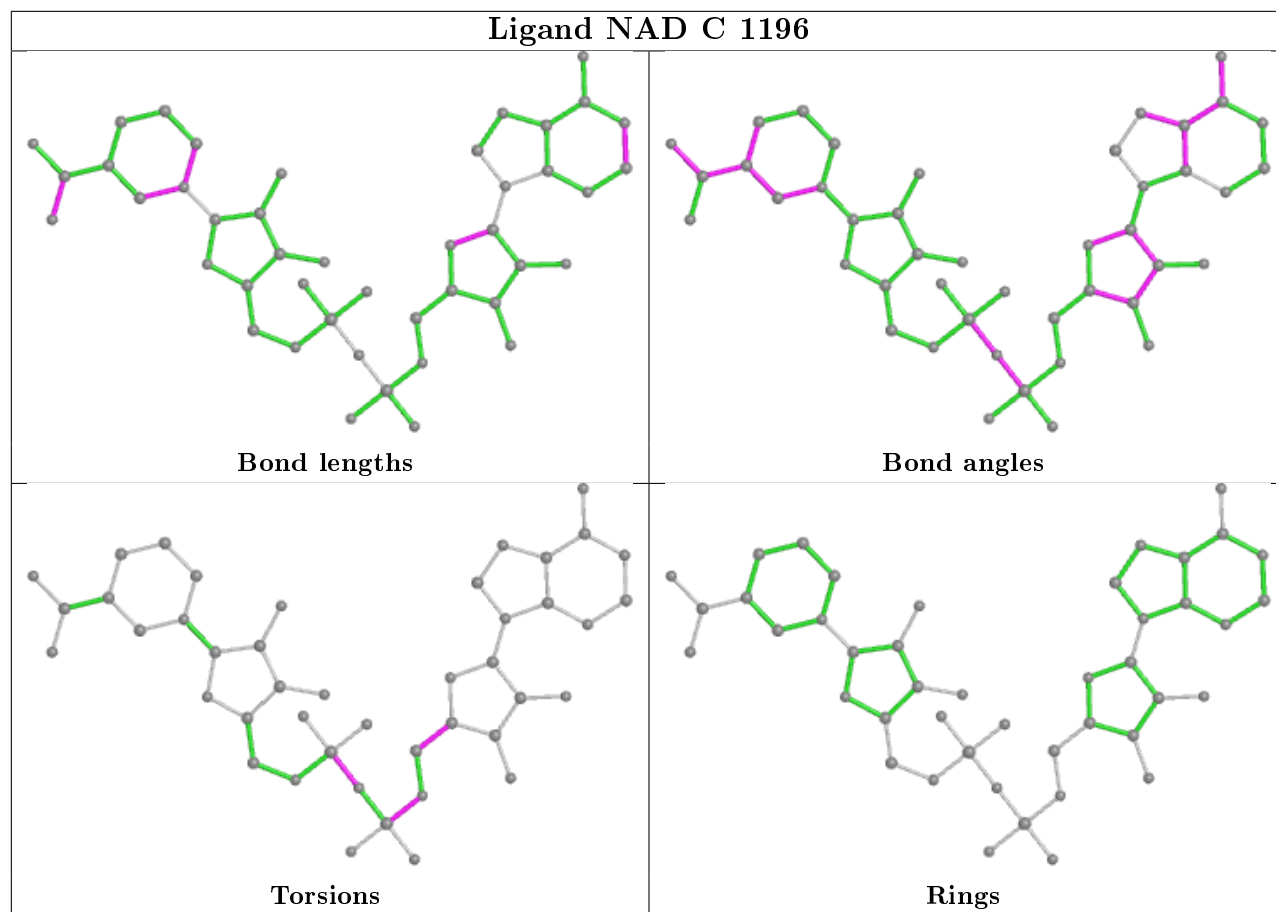
8 monomers are involved in 34 short contacts:

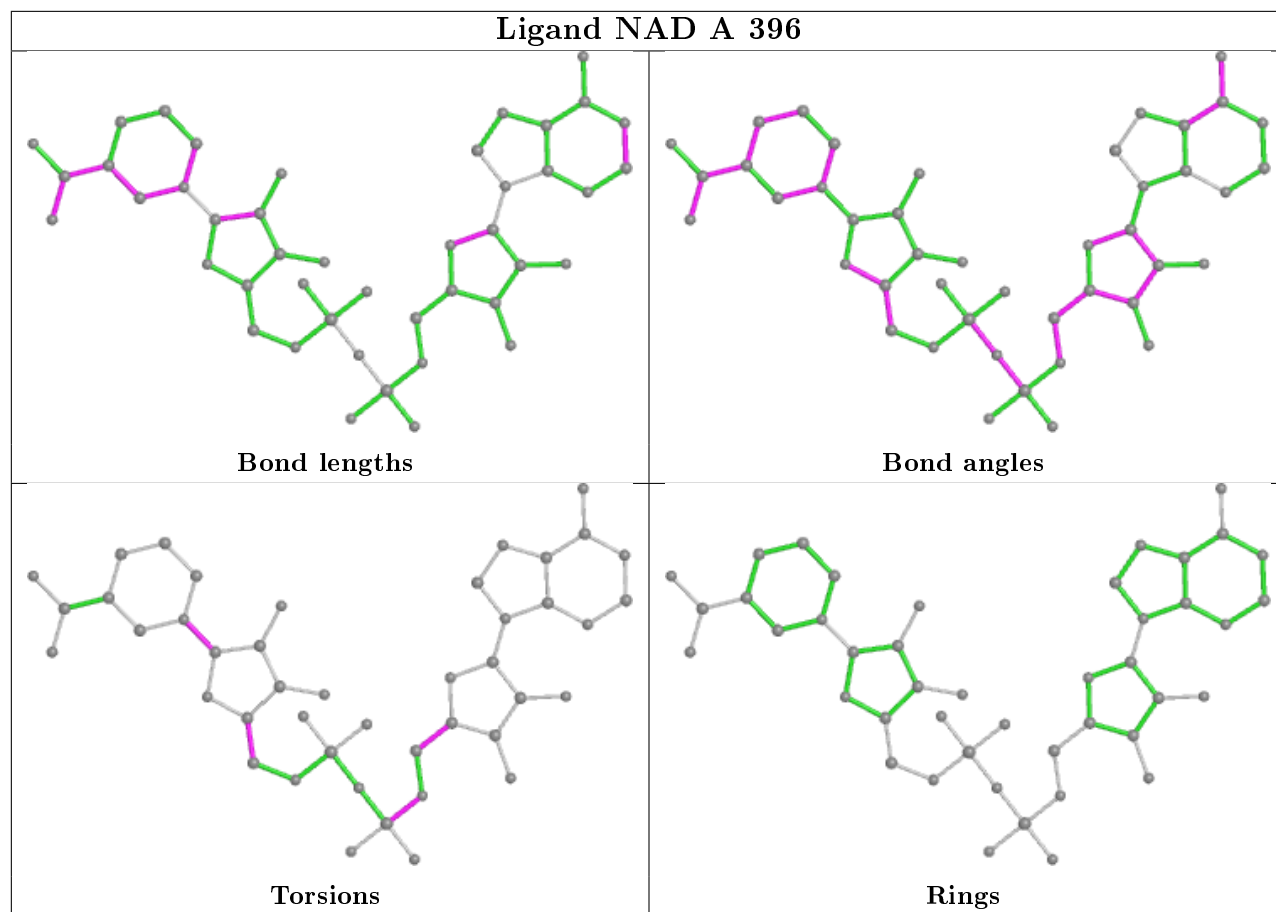
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1596	NAD	9	0
2	D	1595	PO4	2	0
2	B	795	PO4	1	0
3	B	796	NAD	5	0
3	C	1196	NAD	8	0
2	A	395	PO4	1	0
3	A	396	NAD	6	0
2	C	1195	PO4	2	0

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	392/392 (100%)	0.32	23 (5%) 22 25	14, 41, 77, 131	0
1	B	392/392 (100%)	0.46	43 (10%) 5 6	16, 42, 80, 158	0
1	C	392/392 (100%)	0.28	23 (5%) 22 25	7, 38, 71, 131	0
1	D	392/392 (100%)	0.47	33 (8%) 11 12	14, 43, 80, 149	0
All	All	1568/1568 (100%)	0.38	122 (7%) 13 14	7, 41, 77, 158	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	LEU	8.8
1	B	504	GLY	8.2
1	A	115	THR	7.2
1	C	910	LEU	6.5
1	B	507	ILE	6.2
1	D	1318	GLY	5.9
1	B	460	LEU	5.9
1	D	1364	LEU	5.9
1	D	1311	GLY	5.8
1	D	1313	ILE	5.8
1	A	111	GLY	5.7
1	B	516	LEU	5.4
1	A	119	GLU	5.2
1	D	1314	LYS	5.2
1	A	173	GLU	5.0
1	B	513	ILE	4.9
1	D	1290	LEU	4.7
1	A	337	ALA	4.5
1	C	911	GLY	4.5
1	D	1468	ARG	4.5
1	D	1322	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	907	ILE	4.3
1	B	739	LEU	4.3
1	B	505	SER	4.3
1	D	1315	THR	4.1
1	D	1357	SER	3.9
1	D	1347	VAL	3.8
1	B	510	LEU	3.8
1	B	514	LYS	3.7
1	C	1058	GLY	3.7
1	C	916	LEU	3.7
1	A	104	GLY	3.7
1	B	560	TYR	3.6
1	A	170	MET	3.6
1	A	339	LEU	3.5
1	A	340	ILE	3.4
1	B	458	ILE	3.3
1	D	1307	ILE	3.3
1	B	426	GLY	3.2
1	B	566	GLY	3.2
1	B	508	LYS	3.1
1	D	1260	LEU	3.1
1	C	886	VAL	3.1
1	B	614	ALA	3.1
1	C	913	ILE	3.0
1	B	669	ASP	3.0
1	D	1399	PHE	3.0
1	C	947	VAL	3.0
1	B	490	LEU	3.0
1	A	147	VAL	3.0
1	B	599	PHE	2.9
1	B	740	ILE	2.9
1	B	597	ALA	2.9
1	C	962	GLY	2.8
1	A	107	ILE	2.8
1	B	623	GLY	2.8
1	D	1359	GLU	2.8
1	B	743	ILE	2.8
1	A	113	ILE	2.7
1	A	199	PHE	2.7
1	B	545	ILE	2.7
1	C	969	ARG	2.7
1	B	511	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	1360	TYR	2.7
1	C	905	SER	2.7
1	D	1370	MET	2.7
1	A	144	VAL	2.7
1	C	1075	VAL	2.7
1	B	509	GLU	2.7
1	B	506	GLY	2.7
1	B	582	SER	2.7
1	B	660	TYR	2.7
1	D	1310	LEU	2.6
1	D	1319	GLU	2.6
1	B	515	THR	2.6
1	B	512	ASP	2.6
1	C	999	PHE	2.5
1	D	1320	GLY	2.5
1	B	675	VAL	2.5
1	C	1143	ILE	2.5
1	A	114	LYS	2.5
1	A	110	LEU	2.5
1	D	1303	CYS	2.5
1	D	1362	GLY	2.4
1	A	105	SER	2.4
1	C	973	GLU	2.4
1	B	480	ARG	2.4
1	C	1139	LEU	2.4
1	D	1312	ASP	2.4
1	C	827	ILE	2.4
1	D	1317	GLU	2.4
1	A	120	GLY	2.4
1	D	1264	ALA	2.3
1	B	658	GLY	2.3
1	B	501	LEU	2.3
1	A	258	GLY	2.3
1	D	1407	ILE	2.3
1	B	609	ALA	2.3
1	D	1304	GLY	2.3
1	C	923	LEU	2.3
1	B	680	LYS	2.3
1	D	1316	LEU	2.2
1	A	375	ILE	2.2
1	A	276	LEU	2.2
1	B	564	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	805	LEU	2.2
1	A	160	TYR	2.2
1	C	1080	LYS	2.2
1	B	628	THR	2.2
1	D	1464	VAL	2.2
1	B	522	SER	2.1
1	D	1543	ILE	2.1
1	D	1375	ARG	2.1
1	B	735	VAL	2.1
1	D	1469	ASP	2.1
1	C	945	ILE	2.1
1	B	557	SER	2.1
1	B	527	VAL	2.1
1	C	912	ASP	2.1
1	C	1059	ASP	2.0
1	B	624	ASN	2.0
1	D	1369	ARG	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 carbohydrates 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.

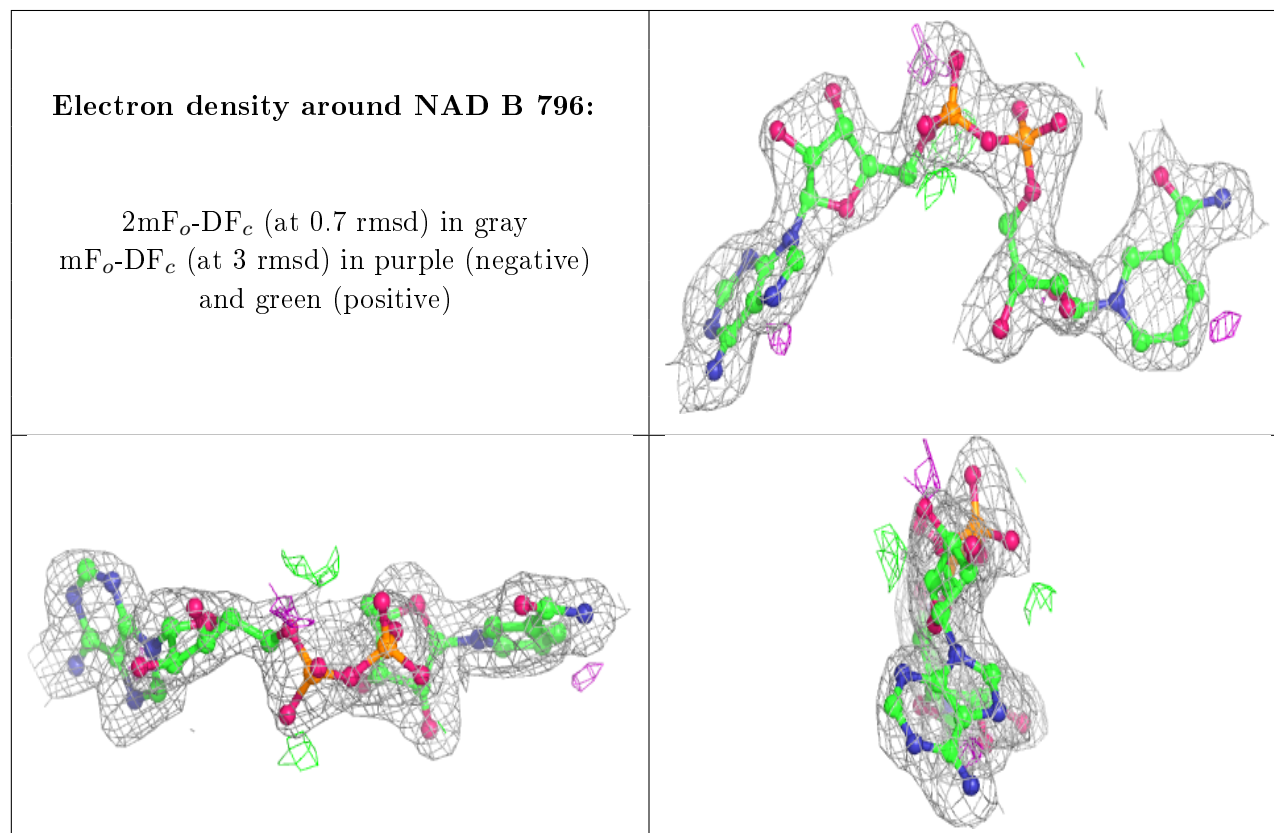
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	C	1195	5/5	0.76	0.24	16,36,53,92	0
4	K	C	1197	1/1	0.80	0.14	60,60,60,60	0
2	PO4	D	1595	5/5	0.92	0.19	28,51,72,87	0
4	K	B	797	1/1	0.93	0.09	67,67,67,67	0
3	NAD	B	796	44/44	0.93	0.11	22,49,65,96	0
3	NAD	A	396	44/44	0.94	0.10	26,49,70,80	0

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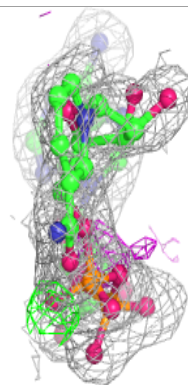
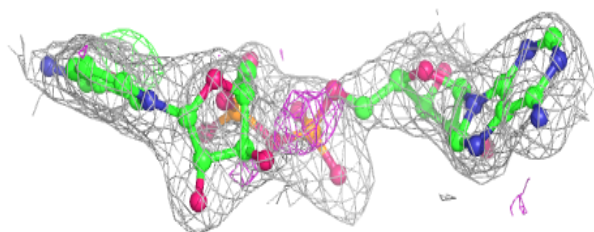
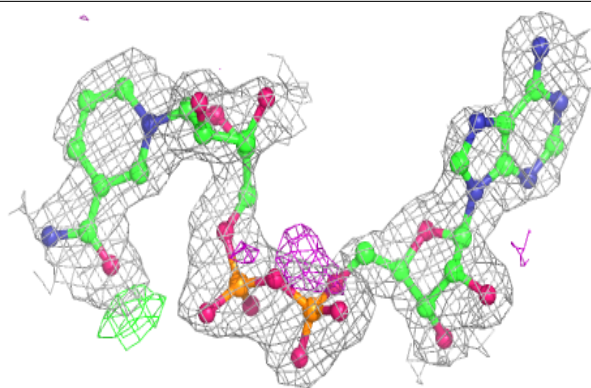
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAD	C	1196	44/44	0.94	0.12	18,43,76,109	0
3	NAD	D	1596	44/44	0.95	0.09	14,45,64,81	0
2	PO4	A	395	5/5	0.98	0.07	22,27,48,78	0
2	PO4	B	795	5/5	0.99	0.10	32,37,61,62	0

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.

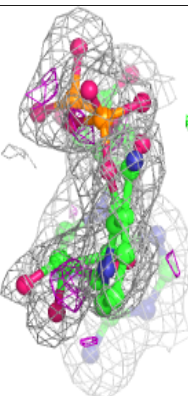
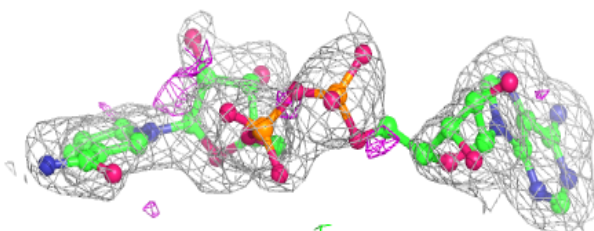
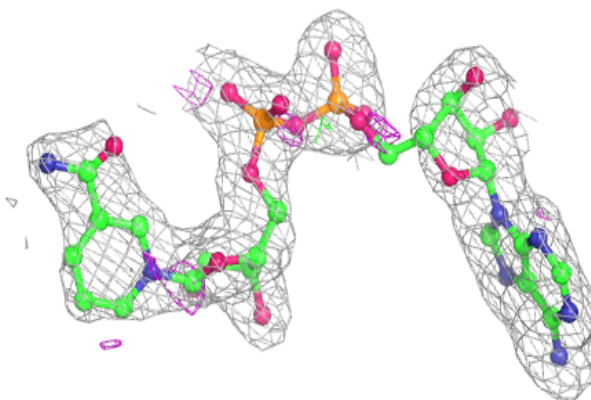


Electron density around NAD A 396:

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

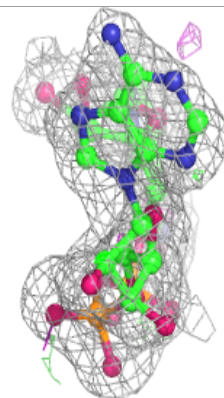
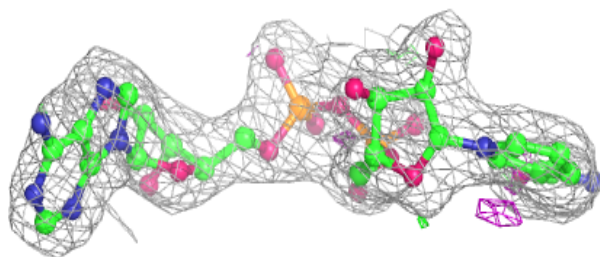
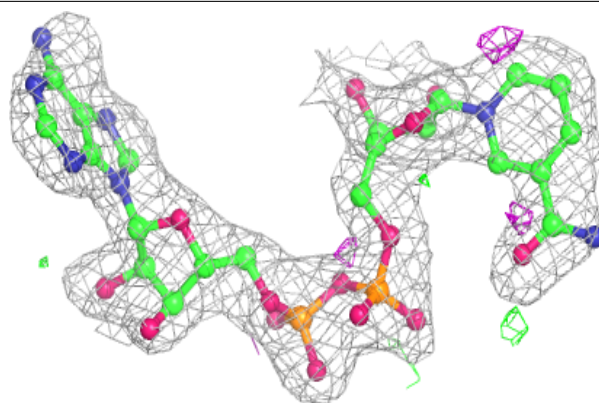
**Electron density around NAD C 1196:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.