



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:29 PM JST

PDB ID : 9X2A / pdb_00009x2a
EMDB ID : EMD-66475
Title : Cryo-EM structure of PsoA in cofactor bound state (PsoA-PKS-II)
Authors : Sun, L.; Bai, L.
Deposited on : 2025-10-04
Resolution : 3.36 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

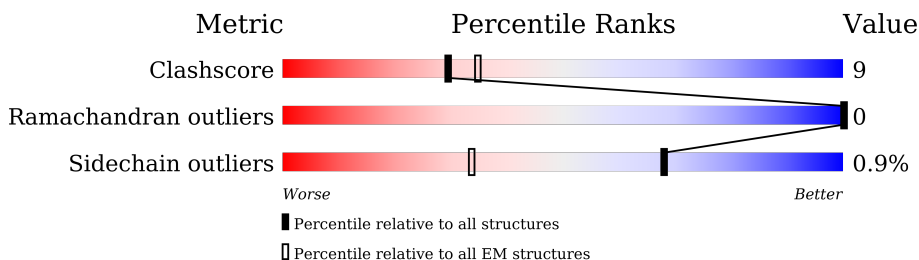
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	4007	
1	B	4007	

2 Entry composition [i](#)

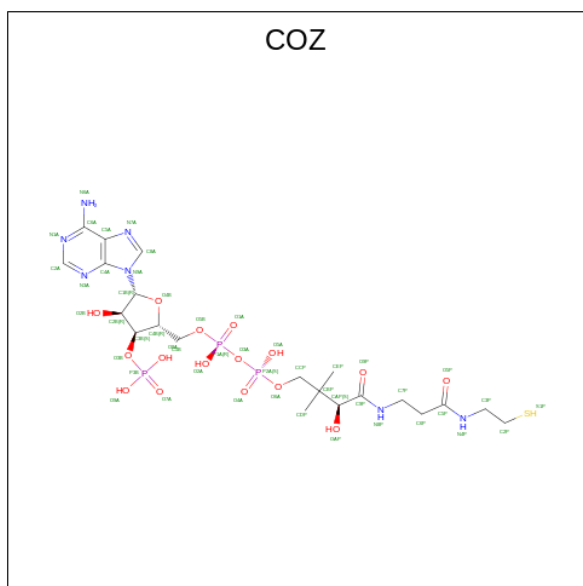
There are 3 unique types of molecules in this entry. The entry contains 72870 atoms, of which 36214 are hydrogens and 0 are deuteriums.

In the tables below, 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 PKS-NRPS hybrid synthetase psoA.

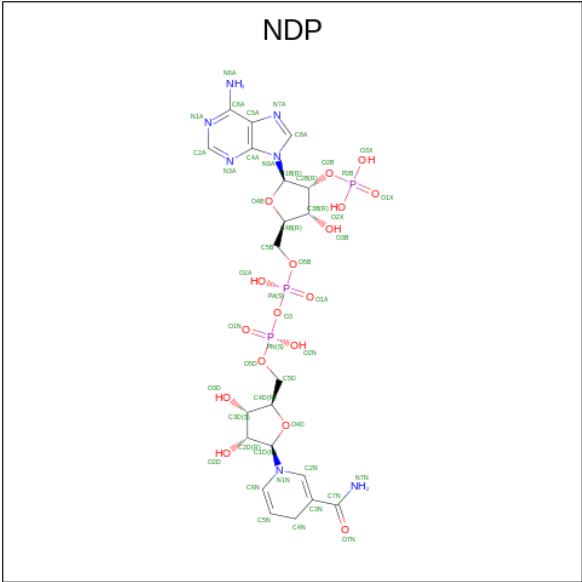
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2382	Total	C	H	N	O	S	0	0
			36281	11461	18049	3198	3492	81		
1	B	2382	Total	C	H	N	O	S	0	0
			36281	11461	18049	3198	3492	81		

- Molecule 2 is COENZYME A (CCD ID: COZ) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
2	A	1	Total	C	H	N	O	P	S	0
			80	21	32	7	16	3	1	
2	B	1	Total	C	H	N	O	P	S	0
			80	21	32	7	16	3	1	

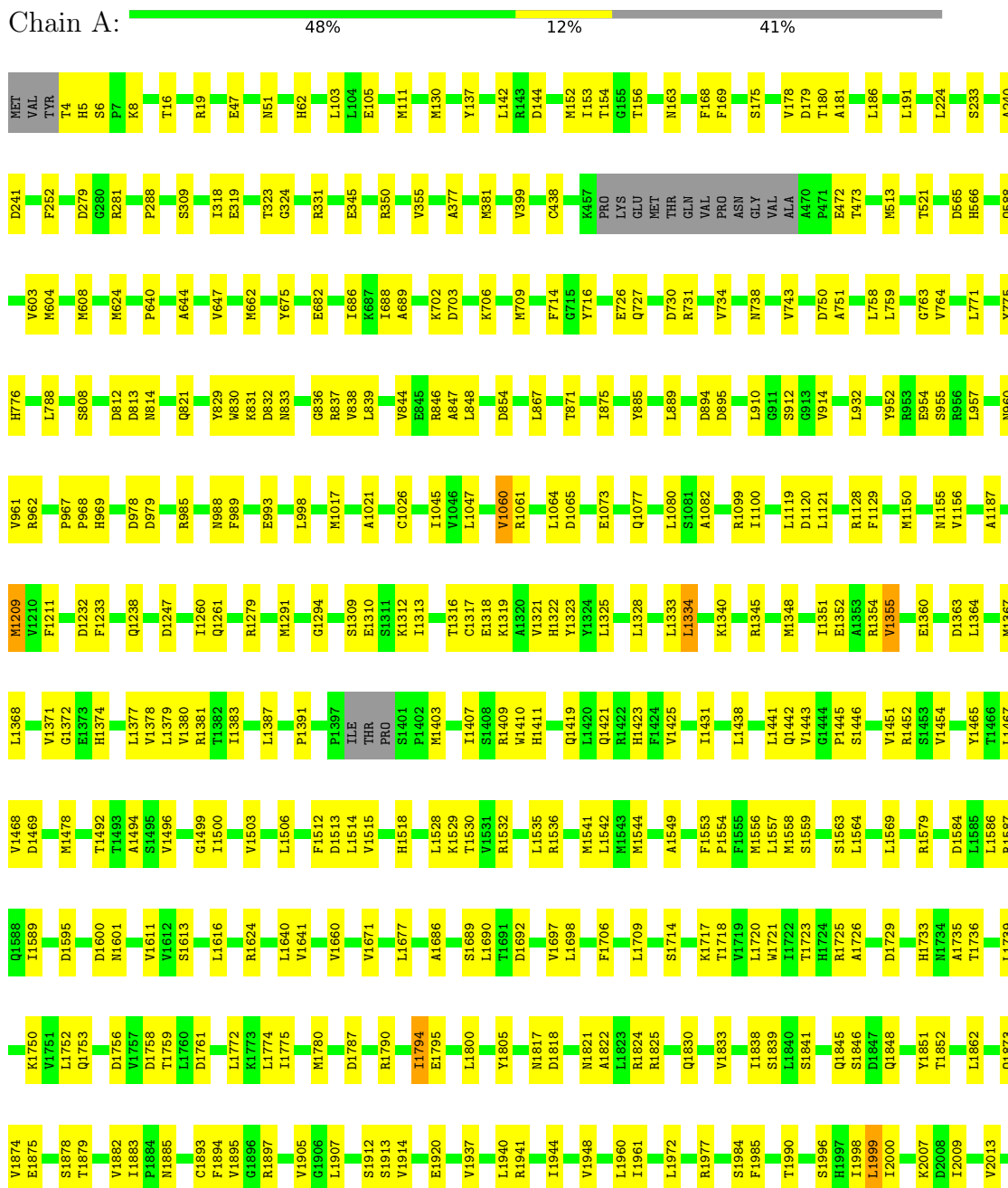
- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: PKS-NRPS hybrid synthetase psoA











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107200	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

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: NDP, COZ

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	0.12	0/18627	0.30	0/25329
1	B	0.12	0/18627	0.30	0/25329
All	All	0.12	0/37254	0.30	0/50658

There are no bond length outliers.

There are no bond angle outliers.

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	18232	18049	18046	345	0
1	B	18232	18049	18046	334	0
2	A	48	32	32	2	0
2	B	48	32	32	2	0
3	A	48	26	26	2	0
3	B	48	26	26	2	0
All	All	36656	36214	36208	672	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 9.

All (672) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:SER:HG	1:A:829:TYR:HH	1.16	0.93
1:B:1061:ARG:NH1	1:B:1077:GLN:OE1	2.02	0.91
1:B:1442:GLN:OE1	1:B:1465:TYR:OH	1.91	0.87
1:A:2007:LYS:NZ	1:B:1247:ASP:OD2	2.08	0.87
1:A:1496:VAL:HG22	1:A:1500:ILE:HD11	1.59	0.85
1:B:1885:ASN:ND2	1:B:2049:ASN:O	2.11	0.83
1:B:1795:GLU:N	1:B:1795:GLU:OE1	2.12	0.83
1:A:1944:ILE:HG23	1:A:2061:LEU:HD21	1.60	0.83
1:B:1841:SER:O	1:B:1852:THR:OG1	1.97	0.83
1:B:1944:ILE:HG23	1:B:2061:LEU:HD21	1.60	0.81
1:B:505:GLU:N	1:B:505:GLU:OE2	2.13	0.81
1:B:1323:TYR:CE1	1:B:1364:LEU:HD22	2.16	0.81
1:A:1830:GLN:OE1	1:A:2112:SER:OG	1.99	0.80
1:A:702:LYS:NZ	1:A:730:ASP:OD1	2.15	0.80
1:A:1841:SER:O	1:A:1852:THR:OG1	1.98	0.80
1:A:1323:TYR:CE1	1:A:1364:LEU:HD22	2.17	0.79
1:A:345:GLU:N	1:A:345:GLU:OE2	2.15	0.79
1:B:759:LEU:HD13	1:B:766:ASN:HD21	1.47	0.79
1:A:1795:GLU:N	1:A:1795:GLU:OE1	2.15	0.79
1:A:776:HIS:NE2	1:A:833:ASN:O	2.15	0.78
1:B:59:ASP:OD1	1:B:60:GLY:N	2.17	0.78
1:A:47:GLU:O	1:A:962:ARG:NH1	2.16	0.78
1:B:1289:GLN:OE1	1:B:1295:ALA:HB3	1.83	0.77
1:A:2264:ILE:HD13	1:A:2361:THR:O	1.84	0.77
1:A:1885:ASN:ND2	1:A:2049:ASN:O	2.18	0.76
1:B:510:ARG:NH2	1:B:935:PRO:O	2.19	0.76
1:A:1411:HIS:ND1	1:A:1446:SER:O	2.19	0.76
1:A:1452:ARG:NH2	1:A:2399:ALA:O	2.19	0.75
1:A:144:ASP:OD1	1:A:955:SER:OG	2.00	0.75
1:B:1841:SER:OG	1:B:1852:THR:OG1	2.03	0.75
1:B:910:LEU:HD23	1:B:914:VAL:HG11	1.68	0.75
1:B:2301:ASP:O	1:B:2361:THR:OG1	2.04	0.75
1:A:2358:GLU:OE1	1:A:2358:GLU:N	2.20	0.75
1:B:1817:ASN:O	1:B:1821:ASN:N	2.19	0.74
1:B:1313:ILE:HG12	1:B:1371:VAL:HG13	1.69	0.74
1:B:1532:ARG:NH2	1:B:1616:LEU:O	2.20	0.74
1:B:2247:GLU:O	1:B:2251:SER:OG	2.05	0.74
1:A:1354:ARG:NH1	1:A:1549:ALA:O	2.21	0.74
1:A:734:VAL:O	1:A:837:ARG:NE	2.21	0.74
1:B:1411:HIS:ND1	1:B:1446:SER:O	2.19	0.74
1:B:1150:MET:CE	1:B:1187:ALA:HB1	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1787:ASP:OD2	1:A:1790:ARG:NE	2.21	0.73
1:A:1553:PHE:CZ	1:A:1557:LEU:HD11	2.23	0.73
1:A:1717:LYS:NZ	1:A:1718:THR:OG1	2.20	0.73
1:B:1874:VAL:N	1:B:1913:SER:O	2.21	0.73
1:B:1830:GLN:OE1	1:B:2112:SER:OG	2.07	0.73
1:A:1407:ILE:HG22	1:A:1411:HIS:CE1	2.24	0.72
1:B:1368:LEU:HD23	1:B:1377:LEU:HD11	1.71	0.72
1:B:1340:LYS:HD3	1:B:1564:LEU:HD21	1.71	0.72
1:A:1232:ASP:OD1	1:A:1233:PHE:N	2.21	0.72
1:B:1026:CYS:SG	1:B:1100:ILE:HD13	2.29	0.72
1:A:309:SER:O	1:A:350:ARG:NH2	2.23	0.71
1:B:309:SER:O	1:B:350:ARG:NH2	2.22	0.71
1:A:1841:SER:OG	1:A:1852:THR:OG1	2.08	0.71
1:A:1325:LEU:HD22	1:A:1334:LEU:HD21	1.72	0.70
1:B:1360:GLU:O	1:B:1364:LEU:N	2.23	0.70
1:B:1764:GLU:OE2	1:B:1764:GLU:N	2.24	0.70
1:A:1733:HIS:O	1:A:1736:THR:OG1	2.09	0.70
1:A:1442:GLN:OE1	1:A:1465:TYR:OH	2.03	0.70
1:B:2317:ASP:OD1	1:B:2318:LYS:N	2.25	0.70
1:A:1960:LEU:HD11	1:A:2013:VAL:HG22	1.73	0.70
1:B:2386:ILE:HG22	1:B:2386:ILE:O	1.90	0.70
1:B:491:ARG:NH2	1:B:548:GLY:O	2.25	0.70
1:B:1232:ASP:OD1	1:B:1233:PHE:N	2.25	0.70
1:B:1322:HIS:ND1	1:B:1351:ILE:O	2.24	0.70
1:B:1407:ILE:HG22	1:B:1411:HIS:CE1	2.27	0.69
1:A:281:ARG:NH1	1:B:168:PHE:O	2.25	0.69
1:A:813:ASP:O	1:A:846:ARG:NH1	2.25	0.69
1:B:702:LYS:NZ	1:B:730:ASP:O	2.23	0.68
1:B:1854:GLU:OE1	1:B:1855:ALA:N	2.27	0.68
1:B:47:GLU:O	1:B:962:ARG:NH1	2.26	0.68
1:B:1875:GLU:OE2	1:B:1897:ARG:NE	2.27	0.68
1:A:1563:SER:O	1:A:1569:LEU:HD11	1.94	0.67
1:B:970:PRO:O	1:B:988:ASN:ND2	2.27	0.67
1:A:1368:LEU:HD23	1:A:1377:LEU:HD11	1.76	0.67
1:A:894:ASP:OD1	1:A:895:ASP:N	2.28	0.67
1:A:1600:ASP:OD1	1:A:1601:ASN:N	2.28	0.67
1:A:1441:LEU:HD13	1:A:1506:LEU:HD21	1.75	0.67
1:A:1360:GLU:O	1:A:1364:LEU:N	2.28	0.66
1:B:1948:VAL:HG22	1:B:2056:VAL:HG11	1.77	0.66
1:A:1817:ASN:O	1:A:1821:ASN:N	2.25	0.66
1:B:957:LEU:HD11	1:B:978:ASP:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1717:LYS:NZ	1:B:1718:THR:OG1	2.28	0.66
1:A:1556:MET:O	1:A:1559:SER:OG	2.14	0.66
1:A:1883:ILE:HD11	1:A:2061:LEU:HD23	1.78	0.66
1:A:988:ASN:OD1	1:A:989:PHE:N	2.28	0.66
1:A:2247:GLU:O	1:A:2251:SER:OG	2.14	0.66
1:B:566:HIS:O	1:B:568:ARG:N	2.28	0.66
1:B:1600:ASP:OD1	1:B:1601:ASN:N	2.30	0.65
1:A:808:SER:OG	1:A:829:TYR:OH	2.01	0.65
1:A:1442:GLN:OE1	1:A:1451:VAL:HG22	1.97	0.65
1:A:1340:LYS:HD3	1:A:1564:LEU:HD21	1.78	0.65
1:A:910:LEU:HD23	1:A:914:VAL:HG11	1.78	0.65
1:A:2301:ASP:O	1:A:2361:THR:OG1	2.15	0.65
1:A:750:ASP:OD1	1:A:751:ALA:N	2.30	0.65
1:A:2262:SER:OG	1:A:2301:ASP:OD1	2.12	0.64
1:B:1445:PRO:HG3	1:B:1467:LEU:HD21	1.79	0.64
1:A:624:MET:HE3	1:A:624:MET:HA	1.79	0.64
1:A:2367:LYS:O	1:A:2369:VAL:HG23	1.98	0.64
1:B:1026:CYS:SG	1:B:1100:ILE:HG21	2.38	0.64
1:A:706:LYS:HE3	1:A:706:LYS:HA	1.80	0.63
1:A:1150:MET:HE1	1:A:1187:ALA:HB1	1.80	0.63
1:A:1322:HIS:ND1	1:A:1351:ILE:O	2.31	0.63
1:A:2248:GLU:OE1	1:A:2249:VAL:HG23	1.99	0.63
1:B:2020:LEU:HD11	1:B:2035:LEU:HD23	1.80	0.63
1:A:1374:HIS:O	1:A:1378:VAL:HG23	1.99	0.62
1:A:1518:HIS:ND1	1:A:1544:MET:SD	2.72	0.62
1:B:882:GLU:N	1:B:882:GLU:OE2	2.33	0.62
1:B:1328:LEU:HD23	1:B:1333:LEU:HD12	1.81	0.62
1:A:233:SER:OG	1:A:323:THR:O	2.17	0.62
1:A:832:ASP:O	1:A:836:GLY:N	2.31	0.62
1:A:1325:LEU:O	1:A:1334:LEU:HD22	1.99	0.62
1:B:1333:LEU:HD22	1:B:1391:PRO:HB3	1.82	0.62
1:A:1875:GLU:OE2	1:A:1897:ARG:NE	2.33	0.62
1:B:218:TYR:O	1:B:222:THR:OG1	2.17	0.62
1:B:964:ARG:HG2	1:B:965:VAL:HG13	1.80	0.62
1:A:1443:VAL:HG13	1:A:1496:VAL:HG21	1.81	0.62
1:A:1723:THR:HG21	1:A:1726:ALA:HB2	1.82	0.62
1:A:2009:ILE:O	1:A:2013:VAL:N	2.33	0.62
1:B:2021:ILE:CG2	1:B:2051:LEU:HD11	2.30	0.62
1:A:1445:PRO:HG3	1:A:1467:LEU:HD21	1.82	0.61
1:B:2056:VAL:HG22	1:B:2061:LEU:HD22	1.81	0.61
1:A:2323:MET:O	1:A:2327:ILE:HD12	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2367:LYS:O	1:B:2369:VAL:HG23	2.00	0.61
1:A:1759:THR:OG1	1:A:1761:ASP:OD1	2.15	0.61
1:B:1441:LEU:HD13	1:B:1506:LEU:HD21	1.82	0.61
1:A:1893:CYS:SG	1:A:1940:LEU:HD23	2.40	0.61
1:B:1787:ASP:OD2	1:B:1790:ARG:NE	2.32	0.61
1:B:2056:VAL:O	1:B:2056:VAL:HG13	2.01	0.61
1:B:821:GLN:O	1:B:825:LEU:HD12	1.99	0.61
1:A:1937:VAL:HG12	1:A:1941:ARG:HD2	1.82	0.61
1:B:1289:GLN:HA	1:B:1806:LEU:HD23	1.83	0.60
1:A:1120:ASP:HB3	1:A:2170:LEU:HD22	1.83	0.60
1:B:2009:ILE:O	1:B:2013:VAL:N	2.34	0.60
1:A:565:ASP:OD1	1:A:566:HIS:N	2.35	0.60
1:B:1714:SER:O	1:B:1750:LYS:NZ	2.35	0.60
1:B:1506:LEU:HD23	1:B:1512:PHE:CZ	2.37	0.60
1:A:1155:ASN:O	1:A:1156:VAL:HG23	2.01	0.59
1:B:616:GLU:OE2	1:B:616:GLU:N	2.31	0.59
1:A:1065:ASP:O	1:A:1065:ASP:OD2	2.20	0.59
1:A:985:ARG:HH22	1:B:1057:LEU:HD21	1.65	0.59
1:A:2209:VAL:HG11	1:A:2212:ILE:HD11	1.84	0.59
1:A:1874:VAL:N	1:A:1913:SER:O	2.33	0.59
1:A:608:MET:HE2	1:A:608:MET:HA	1.85	0.58
1:A:1378:VAL:HG21	1:A:1409:ARG:HH12	1.68	0.58
1:B:1378:VAL:HG21	1:B:1409:ARG:HH12	1.69	0.58
1:B:2021:ILE:HG23	1:B:2051:LEU:HD11	1.85	0.58
1:A:1378:VAL:HG21	1:A:1409:ARG:NH1	2.18	0.58
1:B:1452:ARG:NH2	1:B:2399:ALA:O	2.36	0.58
1:B:1640:LEU:HD23	1:B:1641:VAL:N	2.19	0.58
1:B:1305:ALA:HA	1:B:1602:VAL:HG11	1.85	0.58
1:B:1378:VAL:HG21	1:B:1409:ARG:NH1	2.19	0.58
1:B:1883:ILE:HD11	1:B:2061:LEU:HD23	1.85	0.58
1:B:1023:LYS:NZ	1:B:1216:THR:O	2.31	0.58
1:B:1513:ASP:OD1	1:B:1536:ARG:NE	2.36	0.58
1:A:993:GLU:OE1	1:A:993:GLU:N	2.34	0.58
1:A:1317:CYS:O	1:A:1321:VAL:HG23	2.04	0.58
1:B:1657:GLN:NE2	1:B:1670:ASN:OD1	2.37	0.57
1:A:163:ASN:OD1	1:A:175:SER:OG	2.17	0.57
1:A:1328:LEU:HD23	1:A:1333:LEU:HD12	1.86	0.57
1:B:1893:CYS:SG	1:B:1940:LEU:HD23	2.44	0.57
1:B:2170:LEU:C	1:B:2170:LEU:HD23	2.28	0.57
1:A:2000:ILE:HD11	1:A:2013:VAL:HG23	1.85	0.57
1:A:2172:ARG:HG3	1:A:2182:ILE:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2230:GLU:OE1	1:A:2230:GLU:N	2.37	0.57
1:B:275:CYS:SG	1:B:276:VAL:N	2.77	0.57
1:A:142:LEU:HD21	1:A:152:MET:HE1	1.86	0.57
1:B:1579:ARG:NH2	1:B:1595:ASP:OD1	2.36	0.57
1:B:1478:MET:SD	1:B:1478:MET:N	2.77	0.57
1:B:600:VAL:HG21	1:B:651:LYS:HD3	1.87	0.57
1:A:1948:VAL:HG22	1:A:2056:VAL:HG11	1.86	0.56
1:B:1322:HIS:CG	1:B:1355:VAL:HG23	2.40	0.56
1:B:2192:GLU:N	1:B:2192:GLU:OE1	2.35	0.56
1:B:1291:MET:O	1:B:1294:GLY:N	2.38	0.56
1:B:103:LEU:HD22	1:B:130:MET:CE	2.35	0.56
1:B:750:ASP:OD1	1:B:751:ALA:N	2.38	0.56
1:B:1563:SER:O	1:B:1569:LEU:HD11	2.05	0.56
1:B:1961:ILE:O	1:B:1985:PHE:N	2.39	0.56
1:A:1500:ILE:HG22	1:A:1506:LEU:HB2	1.88	0.56
1:B:1374:HIS:O	1:B:1378:VAL:HG23	2.04	0.56
1:A:998:LEU:HD21	1:A:1047:LEU:CD1	2.35	0.56
1:A:1985:PHE:CZ	1:A:2000:ILE:HD12	2.41	0.56
1:A:1584:ASP:OD1	1:A:1587:ARG:NH2	2.38	0.56
1:B:1640:LEU:HD12	1:B:1684:VAL:HG21	1.88	0.56
1:B:1851:TYR:OH	1:B:1879:THR:O	2.20	0.56
1:A:703:ASP:CG	1:A:703:ASP:O	2.49	0.56
1:B:1801:GLU:O	1:B:1802:ASN:ND2	2.39	0.56
1:B:1832:SER:O	1:B:1835:THR:OG1	2.23	0.56
1:B:1972:LEU:O	1:B:1977:ARG:NE	2.38	0.56
1:A:2165:GLU:OE1	1:A:2165:GLU:N	2.35	0.55
1:B:2262:SER:OG	1:B:2263:SER:N	2.38	0.55
1:A:867:LEU:O	1:A:871:THR:HG22	2.06	0.55
1:A:1334:LEU:HD23	1:A:1352:GLU:OE2	2.06	0.55
1:A:1671:VAL:HG11	1:A:1677:LEU:HD22	1.87	0.55
1:B:2176:LEU:HD21	1:B:2182:ILE:HG22	1.87	0.55
1:A:1321:VAL:HG13	1:A:1553:PHE:CD2	2.40	0.55
1:B:2240:VAL:HG12	1:B:2282:PHE:CE1	2.41	0.55
1:A:1780:MET:SD	1:A:1780:MET:C	2.89	0.55
1:A:1846:SER:OG	1:A:1848:GLN:O	2.24	0.55
1:A:2056:VAL:HG22	1:A:2061:LEU:HD22	1.89	0.55
1:B:734:VAL:O	1:B:837:ARG:NE	2.39	0.55
1:B:1027:ARG:NH2	1:B:1064:LEU:HD23	2.21	0.55
1:A:1532:ARG:NH2	1:A:1616:LEU:O	2.39	0.55
1:A:854:ASP:N	1:A:854:ASP:OD1	2.37	0.55
1:A:2056:VAL:O	1:A:2056:VAL:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:GLU:OE2	1:B:312:GLU:N	2.38	0.55
1:A:1150:MET:CE	1:A:1187:ALA:HB1	2.35	0.55
1:B:813:ASP:O	1:B:846:ARG:NH1	2.35	0.55
1:B:2346:GLU:N	1:B:2346:GLU:OE1	2.40	0.55
1:A:682:GLU:N	1:A:682:GLU:OE1	2.35	0.55
1:B:1496:VAL:HG22	1:B:1500:ILE:HD11	1.89	0.54
1:A:998:LEU:HD21	1:A:1047:LEU:HD11	1.89	0.54
1:A:1333:LEU:HD22	1:A:1391:PRO:HB3	1.88	0.54
1:B:1619:HIS:CB	1:B:1780:MET:HE2	2.38	0.54
1:A:1961:ILE:O	1:A:1985:PHE:N	2.39	0.54
1:B:1553:PHE:CZ	1:B:1557:LEU:HD11	2.42	0.54
1:B:521:THR:HG21	1:B:912:SER:CB	2.37	0.54
1:B:1419:GLN:O	1:B:1423:HIS:ND1	2.41	0.54
1:B:1443:VAL:HG13	1:B:1496:VAL:HG21	1.89	0.54
1:A:1247:ASP:OD2	1:B:2007:LYS:NZ	2.34	0.54
1:A:1383:ILE:O	1:A:1387:LEU:HD12	2.08	0.54
1:A:1313:ILE:HB	1:A:1371:VAL:HG13	1.89	0.54
1:B:1671:VAL:HG11	1:B:1677:LEU:HD22	1.90	0.54
1:A:1407:ILE:HG12	1:A:1558:MET:HE1	1.89	0.54
1:B:2369:VAL:HG22	1:B:2389:PRO:HG3	1.89	0.54
1:A:1940:LEU:N	1:A:2069:ILE:HD11	2.22	0.54
1:B:1150:MET:HE2	1:B:1187:ALA:HB1	1.89	0.54
1:A:1478:MET:SD	1:A:1478:MET:N	2.80	0.53
1:A:2192:GLU:OE1	1:A:2192:GLU:N	2.39	0.53
1:B:521:THR:HG21	1:B:912:SER:HB3	1.89	0.53
1:A:714:PHE:HE1	1:A:764:VAL:HG21	1.73	0.53
1:A:1120:ASP:OD1	1:A:1121:LEU:N	2.42	0.53
1:A:1313:ILE:HG22	1:A:1371:VAL:HA	1.89	0.53
1:A:1379:LEU:HB3	1:A:1383:ILE:HD12	1.89	0.53
1:B:727:GLN:O	1:B:731:ARG:NH1	2.41	0.53
1:B:1985:PHE:CZ	1:B:2000:ILE:HD12	2.43	0.53
1:A:1128:ARG:HD3	1:A:2320:VAL:HG12	1.90	0.53
1:A:513:MET:HE3	1:A:513:MET:HA	1.89	0.53
1:A:1443:VAL:CG1	1:A:1496:VAL:HG21	2.39	0.53
1:B:320:ALA:O	1:B:357:SER:OG	2.20	0.53
1:B:767:ARG:NE	2:B:4101:COZ:O8A	2.41	0.53
1:A:1920:GLU:OE2	1:A:2059:ARG:NH1	2.41	0.53
1:B:725:MET:HE2	1:B:725:MET:N	2.23	0.53
1:B:2185:GLU:OE1	1:B:2201:ARG:NE	2.41	0.53
1:A:1660:VAL:HG23	1:A:1772:LEU:HD21	1.90	0.53
1:B:1990:THR:HG22	1:B:1999:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:HG12	1:A:399:VAL:O	2.09	0.52
1:B:1438:LEU:HD21	1:B:1514:LEU:HD22	1.91	0.52
1:B:2013:VAL:HG11	1:B:2038:ALA:HB1	1.92	0.52
1:A:178:VAL:HG21	1:A:191:LEU:CD1	2.39	0.52
1:A:624:MET:HE3	1:A:624:MET:CA	2.38	0.52
1:A:1468:VAL:HG11	1:A:1500:ILE:HD13	1.91	0.52
1:B:860:GLU:C	1:B:861:ILE:HD13	2.34	0.52
1:B:1694:ASP:OD1	1:B:1694:ASP:C	2.52	0.52
1:B:1882:VAL:HB	1:B:1944:ILE:HG21	1.92	0.52
1:A:1403:MET:O	1:A:1407:ILE:HG13	2.09	0.52
1:B:2133:LEU:HB3	1:B:2212:ILE:HG23	1.92	0.52
1:A:967:PRO:O	1:A:969:HIS:N	2.42	0.52
1:B:2000:ILE:HD11	1:B:2013:VAL:HG23	1.90	0.52
1:B:998:LEU:HD21	1:B:1047:LEU:HD11	1.90	0.52
1:B:1940:LEU:HD13	1:B:2069:ILE:HD12	1.92	0.52
1:B:2056:VAL:CG2	1:B:2061:LEU:HD22	2.39	0.52
1:A:662:MET:SD	1:A:847:ALA:HB1	2.50	0.52
1:A:2021:ILE:CG2	1:A:2051:LEU:HD11	2.40	0.52
1:B:1940:LEU:CA	1:B:2069:ILE:HD11	2.39	0.52
1:A:224:LEU:CD1	1:B:153:ILE:HG21	2.40	0.52
1:A:1824:ARG:O	1:A:1824:ARG:NH1	2.43	0.52
1:B:998:LEU:HD21	1:B:1047:LEU:CD1	2.40	0.52
1:A:1026:CYS:SG	1:A:1100:ILE:HG21	2.50	0.51
1:A:1368:LEU:HA	1:A:1377:LEU:HD21	1.91	0.51
1:A:1541:MET:SD	1:A:1613:SER:N	2.83	0.51
1:B:988:ASN:OD1	1:B:989:PHE:N	2.42	0.51
1:B:1379:LEU:HB3	1:B:1383:ILE:HD12	1.92	0.51
1:A:844:VAL:O	1:A:848:LEU:HD23	2.10	0.51
1:A:1073:GLU:OE2	1:A:1099:ARG:NH1	2.43	0.51
1:A:1387:LEU:HD11	1:A:1557:LEU:HD13	1.91	0.51
1:A:1506:LEU:HD23	1:A:1512:PHE:CZ	2.46	0.51
1:B:1528:LEU:HB2	1:B:1589:ILE:HD13	1.92	0.51
1:A:2262:SER:OG	1:A:2263:SER:N	2.43	0.51
1:B:1383:ILE:O	1:B:1387:LEU:HD12	2.10	0.51
1:A:1720:LEU:HD12	1:A:1721:TRP:N	2.26	0.51
1:B:2161:SER:OG	3:B:4102:NDP:O2B	2.29	0.51
1:B:1940:LEU:N	1:B:2069:ILE:HD11	2.26	0.51
1:A:2125:LEU:O	1:A:2125:LEU:HD23	2.11	0.50
1:B:2136:GLY:O	1:B:2137:LEU:HD12	2.11	0.50
1:A:377:ALA:O	1:A:381:MET:HG3	2.12	0.50
1:A:1209:MET:HE2	1:A:1211:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2088:ALA:O	1:A:2092:VAL:HG23	2.11	0.50
1:A:2125:LEU:HD23	1:A:2125:LEU:C	2.36	0.50
1:B:2240:VAL:HG12	1:B:2282:PHE:CD1	2.46	0.50
1:A:1310:GLU:CD	1:A:1313:ILE:HD11	2.36	0.50
1:A:2195:LEU:HB2	1:A:2249:VAL:HG21	1.94	0.50
1:B:1003:VAL:HG21	1:B:1202:MET:HE1	1.93	0.50
1:B:1825:ARG:HA	1:B:1825:ARG:NE	2.25	0.50
1:A:168:PHE:O	1:B:281:ARG:NH1	2.44	0.50
1:A:1061:ARG:O	1:A:1061:ARG:HG2	2.11	0.50
1:A:472:GLU:OE1	1:A:472:GLU:N	2.44	0.50
1:A:2176:LEU:HD11	1:A:2182:ILE:HG22	1.93	0.50
1:B:825:LEU:HD12	1:B:825:LEU:H	1.77	0.50
1:A:6:SER:OG	1:A:8:LYS:O	2.27	0.50
1:B:1467:LEU:N	1:B:1490:ASP:O	2.40	0.50
1:B:2172:ARG:HG2	1:B:2182:ILE:HG21	1.93	0.50
1:B:759:LEU:O	1:B:763:GLY:N	2.41	0.50
1:A:759:LEU:O	1:A:763:GLY:N	2.40	0.50
1:B:2137:LEU:HD21	1:B:2261:PHE:HE2	1.77	0.49
1:A:2162:ARG:NE	3:A:4102:NDP:O3X	2.45	0.49
1:A:788:LEU:HD23	1:A:788:LEU:O	2.11	0.49
1:A:1309:SER:O	1:A:1313:ILE:HG12	2.12	0.49
1:B:1321:VAL:O	1:B:1325:LEU:HD12	2.12	0.49
1:A:979:ASP:OD2	1:A:979:ASP:C	2.55	0.49
1:A:1500:ILE:HG21	1:A:1506:LEU:HD22	1.95	0.49
1:B:1432:SER:HB2	1:B:1458:LEU:HD11	1.95	0.49
1:A:688:ILE:HD13	1:A:830:TRP:NE1	2.27	0.49
1:A:1421:GLN:O	1:A:1425:VAL:HG23	2.12	0.49
1:A:1752:LEU:HD23	1:A:1753:GLN:N	2.28	0.49
1:A:2312:GLN:OE1	1:A:2312:GLN:C	2.56	0.49
1:A:821:GLN:N	1:A:821:GLN:OE1	2.46	0.49
1:A:2056:VAL:CG2	1:A:2061:LEU:HD22	2.42	0.49
1:B:2386:ILE:O	1:B:2386:ILE:CG2	2.60	0.49
1:A:1279:ARG:HB2	1:A:2333:MET:HE1	1.95	0.49
1:A:1419:GLN:O	1:A:1423:HIS:ND1	2.46	0.49
1:B:967:PRO:N	1:B:968:PRO:CD	2.76	0.49
1:B:979:ASP:C	1:B:979:ASP:OD1	2.56	0.49
1:B:1619:HIS:HB3	1:B:1780:MET:HE2	1.94	0.49
1:A:1045:ILE:HD11	1:A:1082:ALA:CB	2.43	0.49
1:A:2369:VAL:HG22	1:A:2389:PRO:HG3	1.94	0.49
1:A:647:VAL:HG13	1:A:675:TYR:CE2	2.47	0.48
1:B:1338:ALA:HB1	1:B:1345:ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1874:VAL:HG22	1:B:1894:PHE:CD1	2.48	0.48
1:A:1940:LEU:CA	1:A:2069:ILE:HD11	2.43	0.48
1:A:967:PRO:N	1:A:968:PRO:CD	2.76	0.48
1:A:1328:LEU:HB2	1:A:1334:LEU:HD13	1.95	0.48
1:A:1506:LEU:HD23	1:A:1512:PHE:CE2	2.49	0.48
1:A:1541:MET:O	1:A:1542:LEU:HD23	2.13	0.48
1:A:1714:SER:O	1:A:1750:LYS:NZ	2.46	0.48
1:A:1883:ILE:CD1	1:A:2061:LEU:HD23	2.43	0.48
1:B:1262:ILE:C	1:B:1263:GLU:OE1	2.56	0.48
1:B:2020:LEU:HD23	1:B:2021:ILE:N	2.28	0.48
1:A:1328:LEU:HD13	1:A:1334:LEU:HD13	1.96	0.48
1:B:822:ASP:HA	1:B:825:LEU:HD13	1.96	0.48
1:B:1963:GLU:N	1:B:1985:PHE:O	2.46	0.48
1:B:2020:LEU:HD22	1:B:2022:HIS:CD2	2.48	0.48
1:B:240:ALA:HB1	1:B:324:GLY:O	2.13	0.48
1:B:583:TRP:O	1:B:586:MET:HE2	2.13	0.48
1:A:1874:VAL:HG22	1:A:1894:PHE:CD1	2.47	0.48
1:B:894:ASP:OD1	1:B:895:ASP:N	2.45	0.48
1:B:2048:PHE:HA	1:B:2051:LEU:HD12	1.96	0.48
1:A:1972:LEU:O	1:A:1977:ARG:NE	2.46	0.48
1:A:1729:ASP:OD1	1:A:1729:ASP:C	2.56	0.48
1:A:2144:SER:OG	1:A:2341:HIS:NE2	2.43	0.47
1:B:647:VAL:HG13	1:B:675:TYR:CE1	2.48	0.47
1:A:318:ILE:HG23	1:A:355:VAL:HG23	1.96	0.47
1:A:1862:LEU:HD12	1:A:2127:SER:CB	2.44	0.47
1:A:1944:ILE:HG23	1:A:2061:LEU:CD2	2.39	0.47
1:A:1017:MET:CE	1:A:1080:LEU:HD22	2.44	0.47
1:A:1500:ILE:HG22	1:A:1500:ILE:O	2.14	0.47
1:B:1017:MET:CE	1:B:1080:LEU:HD22	2.44	0.47
1:A:1319:LYS:HA	1:A:1355:VAL:HG21	1.96	0.47
1:B:1045:ILE:HD11	1:B:1082:ALA:CB	2.44	0.47
1:B:1873:GLN:OE1	1:B:1914:VAL:HG22	2.13	0.47
1:B:1944:ILE:O	1:B:1948:VAL:HG23	2.14	0.47
1:A:1689:SER:O	1:A:1690:LEU:HD23	2.15	0.47
1:A:2020:LEU:HD12	1:A:2039:LEU:HD11	1.95	0.47
1:A:137:TYR:HD2	1:A:156:THR:HG22	1.78	0.47
1:A:1328:LEU:CB	1:A:1334:LEU:HD13	2.45	0.47
1:A:2032:PHE:CD1	1:A:2032:PHE:C	2.93	0.47
1:B:1923:ILE:HD12	1:B:2062:LEU:HG	1.96	0.47
1:A:288:PRO:O	1:A:331:ARG:NH1	2.45	0.47
1:A:1438:LEU:HD21	1:A:1514:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1692:ASP:OD2	1:A:1721:TRP:NE1	2.46	0.47
1:B:964:ARG:HG2	1:B:965:VAL:N	2.29	0.47
1:B:1325:LEU:HD11	1:B:1553:PHE:CD1	2.49	0.47
1:B:1325:LEU:HD13	1:B:1351:ILE:HG22	1.97	0.47
1:B:1347:LEU:HD21	1:B:1552:ARG:HD3	1.95	0.47
1:B:1354:ARG:NH1	1:B:1549:ALA:O	2.48	0.47
1:B:1937:VAL:HG12	1:B:1941:ARG:HD2	1.96	0.47
1:A:1312:LYS:O	1:A:1316:THR:OG1	2.27	0.47
1:B:1936:PHE:CD1	1:B:2069:ILE:HG21	2.50	0.47
1:B:1334:LEU:HB3	1:B:1348:MET:HE3	1.97	0.47
1:B:1438:LEU:HD21	1:B:1514:LEU:CD2	2.45	0.47
1:A:186:LEU:HD23	1:A:438:CYS:HB2	1.96	0.47
1:A:1238:GLN:OE1	1:A:1845:GLN:NE2	2.43	0.47
1:A:2314:SER:OG	1:A:2321:SER:OG	2.20	0.47
1:B:288:PRO:O	1:B:331:ARG:NH1	2.47	0.47
1:B:400:LYS:HD2	1:B:400:LYS:O	2.14	0.47
1:B:1758:ASP:OD1	1:B:1758:ASP:N	2.42	0.47
1:A:588:GLN:HG3	1:A:624:MET:HE1	1.97	0.46
1:A:604:MET:HE1	1:A:644:ALA:HA	1.97	0.46
1:A:738:ASN:ND2	2:A:4101:COZ:O9P	2.48	0.46
1:A:871:THR:HG21	1:A:885:TYR:CE2	2.50	0.46
1:B:1155:ASN:O	1:B:1156:VAL:HG23	2.15	0.46
1:A:1541:MET:SD	1:A:1613:SER:OG	2.69	0.46
1:A:1686:ALA:CB	1:A:1775:ILE:HD11	2.45	0.46
1:B:1338:ALA:HB2	1:B:1348:MET:SD	2.55	0.46
1:B:1879:THR:HG22	1:B:2105:VAL:CG2	2.45	0.46
1:A:153:ILE:HG23	1:A:154:THR:HG23	1.97	0.46
1:B:203:ILE:HG22	1:B:204:SER:N	2.31	0.46
1:B:1962:TYR:O	1:B:2023:MET:HE3	2.15	0.46
1:A:758:LEU:HD23	1:A:758:LEU:O	2.15	0.46
1:A:1368:LEU:HD13	1:A:1381:ARG:NE	2.31	0.46
1:A:2120:VAL:HG21	1:A:2345:ALA:CB	2.46	0.46
1:B:1113:GLY:O	1:B:1115:ARG:N	2.49	0.46
1:B:1368:LEU:HA	1:B:1377:LEU:HD21	1.97	0.46
1:B:1512:PHE:HE2	1:B:1534:LEU:HD22	1.80	0.46
1:B:1771:PHE:O	1:B:1775:ILE:HG12	2.16	0.46
1:B:1161:VAL:HG21	1:B:1181:CYS:SG	2.55	0.46
1:A:180:THR:O	1:A:181:ALA:HB3	2.16	0.46
1:B:1443:VAL:HG12	1:B:1519:LYS:HD2	1.96	0.46
1:B:1536:ARG:NH1	1:B:1789:THR:OG1	2.49	0.46
1:A:2048:PHE:HA	1:A:2051:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1660:VAL:HG23	1:B:1772:LEU:HD21	1.98	0.46
1:B:2261:PHE:CD1	1:B:2300:ILE:HD11	2.51	0.46
1:A:1150:MET:HE1	1:A:1187:ALA:CB	2.44	0.46
1:A:2392:ALA:O	1:A:2396:ALA:N	2.49	0.46
1:B:1527:ALA:O	1:B:1531:VAL:HG23	2.16	0.46
1:B:1905:VAL:CG1	1:B:2066:LEU:HD11	2.45	0.46
1:A:51:ASN:N	1:A:961:VAL:O	2.48	0.46
1:B:318:ILE:CG2	1:B:355:VAL:HG23	2.46	0.46
1:B:623:ILE:CD1	1:B:641:VAL:HG13	2.45	0.46
1:B:1434:GLN:O	1:B:1435:HIS:ND1	2.49	0.46
1:A:812:ASP:O	1:A:814:ASN:ND2	2.49	0.45
1:A:1077:GLN:N	1:A:1077:GLN:OE1	2.49	0.45
1:A:1528:LEU:HB2	1:A:1589:ILE:HD13	1.98	0.45
1:A:2275:ASN:OD1	1:A:2276:TYR:N	2.49	0.45
1:B:696:THR:OG1	1:B:780:MET:HE1	2.16	0.45
1:B:787:TYR:CZ	1:B:791:ILE:HD11	2.52	0.45
1:B:233:SER:OG	1:B:323:THR:O	2.32	0.45
1:B:1944:ILE:HG23	1:B:2061:LEU:CD2	2.40	0.45
1:B:2217:MET:HE1	3:B:4102:NDP:H2D	1.99	0.45
1:B:107:VAL:HG21	1:B:165:LEU:HD13	1.98	0.45
1:B:1118:GLU:OE1	1:B:1118:GLU:N	2.50	0.45
1:B:1878:SER:O	1:B:1911:ASN:ND2	2.49	0.45
1:A:241:ASP:OD2	1:A:241:ASP:N	2.49	0.45
1:A:319:GLU:O	1:A:319:GLU:HG3	2.15	0.45
1:A:716:TYR:OH	1:A:837:ARG:NH1	2.45	0.45
1:A:1554:PRO:O	1:A:1558:MET:HG3	2.16	0.45
1:A:1825:ARG:HA	1:A:1825:ARG:NE	2.31	0.45
1:A:2125:LEU:HD21	1:A:2348:ILE:HG21	1.98	0.45
1:B:272:ARG:NH1	1:B:443:GLU:OE2	2.34	0.45
1:B:1120:ASP:OD2	1:B:1121:LEU:N	2.50	0.45
1:B:1818:ASP:HA	1:B:1821:ASN:HB2	1.98	0.45
1:A:521:THR:HG21	1:A:912:SER:HB3	1.98	0.45
1:A:1379:LEU:CB	1:A:1383:ILE:HD12	2.47	0.45
1:A:1729:ASP:OD1	1:A:1729:ASP:O	2.34	0.45
1:A:1940:LEU:HD12	1:A:2065:ALA:HB1	1.98	0.45
1:A:2255:LEU:H	1:A:2255:LEU:HD12	1.82	0.45
1:A:1882:VAL:HB	1:A:1944:ILE:HG21	1.99	0.45
1:B:1685:GLU:C	1:B:1685:GLU:CD	2.84	0.45
1:B:2091:LEU:HD22	1:B:2105:VAL:HG22	1.99	0.45
1:A:2020:LEU:HD23	1:A:2021:ILE:N	2.32	0.45
1:B:1318:GLU:O	1:B:1319:LYS:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1905:VAL:HG11	1:B:2066:LEU:HD11	1.97	0.45
1:A:1387:LEU:HD11	1:A:1557:LEU:CD1	2.47	0.45
1:A:2333:MET:HE3	1:A:2364:GLU:HB2	1.98	0.45
1:B:399:VAL:HG12	1:B:399:VAL:O	2.16	0.45
1:B:861:ILE:HD13	1:B:861:ILE:N	2.32	0.45
1:A:771:LEU:HD11	2:A:4101:COZ:H21	1.98	0.45
1:A:2141:ILE:O	1:A:2145:ILE:HG12	2.17	0.45
1:B:1322:HIS:CG	1:B:1351:ILE:O	2.70	0.45
1:B:2230:GLU:N	1:B:2230:GLU:OE1	2.49	0.45
1:A:1260:ILE:HG22	1:A:1261:GLN:N	2.31	0.44
1:A:1725:ARG:N	1:A:1756:ASP:OD1	2.50	0.44
1:A:1998:ILE:HG22	1:A:1999:LEU:N	2.32	0.44
1:B:1027:ARG:HH21	1:B:1064:LEU:HD23	1.82	0.44
1:B:1515:VAL:HG23	1:B:1535:LEU:HD21	1.98	0.44
1:B:2236:MET:O	1:B:2240:VAL:HG22	2.17	0.44
1:A:4:THR:HG22	1:A:5:HIS:N	2.33	0.44
1:B:1318:GLU:HB3	1:B:1355:VAL:HG22	1.99	0.44
1:A:2239:LYS:O	1:A:2243:SER:OG	2.33	0.44
1:B:691:TYR:CD2	1:B:790:ALA:HB1	2.51	0.44
1:B:821:GLN:OE1	1:B:821:GLN:N	2.50	0.44
1:B:1379:LEU:CB	1:B:1383:ILE:HD12	2.48	0.44
1:A:889:LEU:HD21	1:A:895:ASP:OD2	2.18	0.44
1:A:1129:PHE:CZ	1:A:1187:ALA:HB2	2.52	0.44
1:A:1345:ARG:HA	1:A:1348:MET:HB2	1.99	0.44
1:A:2120:VAL:HG21	1:A:2345:ALA:HB3	1.98	0.44
1:A:714:PHE:O	1:A:743:VAL:HG22	2.18	0.44
1:A:1579:ARG:NH2	1:A:1595:ASP:OD1	2.50	0.44
1:B:2032:PHE:CD1	1:B:2032:PHE:C	2.95	0.44
1:A:1984:SER:N	1:A:1996:SER:OG	2.49	0.44
1:A:2386:ILE:HG22	1:A:2386:ILE:O	2.17	0.44
1:B:572:ILE:HD11	1:B:857:LEU:HD23	1.99	0.44
1:B:2323:MET:O	1:B:2327:ILE:HG12	2.17	0.44
1:A:19:ARG:NH2	1:A:105:GLU:OE1	2.50	0.44
1:A:1431:ILE:HD13	1:A:1514:LEU:HD13	2.00	0.44
1:A:1895:VAL:HG22	1:A:1905:VAL:HG23	2.00	0.44
1:A:1990:THR:HG22	1:A:1999:LEU:CD1	2.47	0.44
1:B:1355:VAL:HG12	1:B:1357:SER:H	1.83	0.44
1:A:1334:LEU:HG	1:A:1348:MET:SD	2.58	0.44
1:A:1374:HIS:O	1:A:1378:VAL:N	2.39	0.44
1:A:2388:ASP:HB2	1:A:2391:ALA:HB2	2.00	0.44
1:B:966:ASP:N	1:B:966:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1842:ARG:NH1	1:B:1880:GLU:OE1	2.49	0.44
1:A:1291:MET:O	1:A:1294:GLY:N	2.51	0.44
1:A:1363:ASP:O	1:A:1367:MET:HG2	2.17	0.44
1:A:1513:ASP:OD1	1:A:1536:ARG:NE	2.50	0.44
1:B:832:ASP:O	1:B:836:GLY:N	2.44	0.44
1:B:846:ARG:NE	1:B:850:GLU:OE2	2.39	0.44
1:B:1260:ILE:HG22	1:B:1261:GLN:N	2.33	0.44
1:A:1774:LEU:C	1:A:1774:LEU:HD23	2.42	0.43
1:B:428:VAL:HG12	1:B:429:ASN:N	2.32	0.43
1:B:1800:LEU:HD21	1:B:1805:TYR:CE2	2.53	0.43
1:A:2260:PHE:HB2	1:A:2299:VAL:HG22	1.98	0.43
1:A:2266:VAL:HA	1:A:2277:VAL:HG13	2.00	0.43
1:B:330:PRO:HA	1:B:399:VAL:HG22	2.01	0.43
1:A:1492:THR:HG21	1:A:1503:VAL:CG1	2.49	0.43
1:A:1758:ASP:OD1	1:A:1758:ASP:N	2.42	0.43
1:A:2240:VAL:HG13	1:A:2282:PHE:CZ	2.53	0.43
1:B:1324:TYR:HD1	1:B:1388:LEU:HD12	1.82	0.43
1:B:1940:LEU:HD12	1:B:2065:ALA:HB1	1.99	0.43
1:B:1960:LEU:HD11	1:B:2013:VAL:HG22	2.01	0.43
1:A:103:LEU:HD22	1:A:130:MET:CE	2.47	0.43
1:A:848:LEU:HD21	1:A:875:ILE:CD1	2.48	0.43
1:A:1021:ALA:HB1	1:A:1060:VAL:HG21	1.99	0.43
1:A:1800:LEU:HD11	1:A:1805:TYR:CE1	2.53	0.43
1:B:631:ARG:NE	1:B:634:GLU:OE2	2.47	0.43
1:B:1500:ILE:O	1:B:1500:ILE:CG2	2.66	0.43
1:B:1724:HIS:CD2	1:B:1760:LEU:HD21	2.53	0.43
1:B:1854:GLU:OE1	1:B:1855:ALA:C	2.62	0.43
1:B:2199:ARG:HA	1:B:2202:ILE:HG22	2.01	0.43
1:A:521:THR:HG21	1:A:912:SER:CB	2.48	0.43
1:A:1883:ILE:HD12	1:A:1907:LEU:HD13	2.00	0.43
1:A:2013:VAL:HG11	1:A:2038:ALA:HB1	1.99	0.43
1:B:1291:MET:HE1	1:B:1597:ILE:HG21	1.99	0.43
1:B:1340:LYS:CD	1:B:1564:LEU:HD21	2.46	0.43
1:B:2047:ALA:O	1:B:2051:LEU:N	2.50	0.43
1:A:1529:LYS:NZ	1:A:1589:ILE:O	2.47	0.43
1:A:1851:TYR:OH	1:A:1879:THR:O	2.33	0.43
1:B:521:THR:HG21	1:B:912:SER:HB2	2.01	0.43
1:B:1020:GLU:OE1	1:B:1171:ILE:HG23	2.19	0.43
1:B:1965:ASP:OD2	1:B:1967:HIS:N	2.52	0.43
1:B:2236:MET:O	1:B:2237:LYS:C	2.61	0.43
1:B:365:THR:O	1:B:369:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1292:LEU:HD23	1:B:1292:LEU:O	2.18	0.43
1:B:1403:MET:O	1:B:1407:ILE:HG13	2.18	0.43
1:B:1794:ILE:HD12	1:B:1794:ILE:H	1.83	0.43
1:A:179:ASP:O	1:B:177:SER:OG	2.31	0.43
1:A:726:GLU:OE1	1:A:726:GLU:C	2.61	0.43
1:A:1321:VAL:CG1	1:A:1553:PHE:CB	2.97	0.43
1:A:1706:PHE:HA	1:A:1709:LEU:HD12	2.00	0.43
1:B:385:THR:HG22	1:B:386:ILE:N	2.34	0.43
1:B:767:ARG:NH1	2:B:4101:COZ:O1A	2.52	0.43
1:B:1079:THR:O	1:B:1079:THR:HG23	2.18	0.43
1:B:1300:ALA:O	1:B:1599:LEU:HD12	2.19	0.43
1:B:1656:ILE:O	1:B:1660:VAL:HG12	2.19	0.43
1:A:2225:ILE:HD12	1:A:2225:ILE:H	1.84	0.43
1:B:1223:SER:C	1:B:1253:SER:HG	2.26	0.43
1:B:1891:LEU:CD1	1:B:1909:THR:HG22	2.49	0.43
1:A:16:THR:HG22	1:A:252:PHE:CD1	2.54	0.42
1:B:1443:VAL:CG1	1:B:1496:VAL:HG21	2.49	0.42
1:B:1862:LEU:HD12	1:B:2127:SER:CB	2.49	0.42
1:A:111:MET:HE1	1:A:169:PHE:CD1	2.53	0.42
1:B:61:GLU:OE1	1:B:225:HIS:NE2	2.49	0.42
1:B:2300:ILE:CG2	1:B:2347:ALA:HB2	2.49	0.42
1:A:1961:ILE:HD13	1:A:1972:LEU:HD13	2.01	0.42
1:B:1064:LEU:O	1:B:1065:ASP:HB3	2.19	0.42
1:B:2365:THR:O	1:B:2365:THR:OG1	2.36	0.42
1:A:1310:GLU:O	1:A:1313:ILE:HG13	2.19	0.42
1:A:1873:GLN:OE1	1:A:1914:VAL:HG22	2.20	0.42
1:B:1547:THR:OG1	1:B:1609:SER:OG	2.20	0.42
1:A:240:ALA:HB1	1:A:324:GLY:O	2.19	0.42
1:A:1318:GLU:O	1:A:1321:VAL:N	2.53	0.42
1:A:1515:VAL:HG23	1:A:1535:LEU:HD21	2.00	0.42
1:A:2020:LEU:HD22	1:A:2022:HIS:ND1	2.34	0.42
1:B:758:LEU:HD23	1:B:758:LEU:O	2.19	0.42
1:B:811:TYR:N	1:B:811:TYR:CD1	2.85	0.42
1:B:1247:ASP:OD1	1:B:1247:ASP:C	2.62	0.42
1:B:1321:VAL:HG13	1:B:1553:PHE:CB	2.50	0.42
1:B:2259:LEU:HD21	1:B:2347:ALA:HB1	2.01	0.42
1:B:2388:ASP:HB2	1:B:2391:ALA:HB2	2.01	0.42
1:A:1697:VAL:HG11	1:A:1709:LEU:HD21	2.01	0.42
1:B:1282:TYR:HB2	1:B:1813:ASP:HB3	2.01	0.42
1:B:1440:ILE:HD11	1:B:1458:LEU:HD22	2.02	0.42
1:A:838:VAL:C	1:A:839:LEU:HD12	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1794:ILE:H	1:A:1794:ILE:HD12	1.85	0.42
1:A:1833:VAL:HA	1:A:1838:ILE:HD12	2.01	0.42
1:B:623:ILE:HD13	1:B:641:VAL:HG13	2.00	0.42
1:A:1310:GLU:HA	1:A:1313:ILE:HG12	2.02	0.42
1:A:1379:LEU:O	1:A:1380:VAL:C	2.63	0.42
1:B:957:LEU:HD12	1:B:977:PRO:HB2	2.02	0.42
1:B:2198:LEU:O	1:B:2202:ILE:HG22	2.19	0.42
1:A:727:GLN:O	1:A:731:ARG:NH1	2.53	0.42
1:A:1064:LEU:HD12	1:A:1065:ASP:N	2.35	0.42
1:A:1372:GLY:O	1:A:1377:LEU:HD22	2.20	0.42
1:A:1879:THR:HG22	1:A:2105:VAL:CG2	2.50	0.42
1:A:1698:LEU:HD12	1:A:1735:ALA:HB3	2.00	0.41
1:B:178:VAL:HG21	1:B:191:LEU:CD1	2.49	0.41
1:B:1325:LEU:HD22	1:B:1351:ILE:HB	2.02	0.41
1:B:1379:LEU:O	1:B:1380:VAL:C	2.62	0.41
1:B:1452:ARG:NH2	1:B:1485:ASP:OD2	2.53	0.41
1:A:137:TYR:CD2	1:A:156:THR:HG22	2.54	0.41
1:A:1839:SER:HA	1:A:1912:SER:HA	2.02	0.41
1:B:812:ASP:OD1	1:B:813:ASP:N	2.53	0.41
1:B:1374:HIS:O	1:B:1378:VAL:N	2.41	0.41
1:B:1543:MET:O	1:B:1611:VAL:N	2.39	0.41
1:B:2136:GLY:N	1:B:2160:THR:O	2.43	0.41
1:A:2047:ALA:O	1:A:2051:LEU:N	2.54	0.41
1:A:2140:HIS:HA	1:A:2143:GLN:HG3	2.03	0.41
1:A:2170:LEU:HD23	1:A:2170:LEU:C	2.45	0.41
1:B:565:ASP:OD1	1:B:566:HIS:N	2.53	0.41
1:B:734:VAL:O	1:B:734:VAL:HG23	2.20	0.41
1:A:1438:LEU:HD21	1:A:1514:LEU:CD2	2.51	0.41
1:A:1905:VAL:HG11	1:A:2066:LEU:HD21	2.03	0.41
1:B:682:GLU:OE1	1:B:682:GLU:N	2.42	0.41
1:B:690:TYR:O	1:B:694:VAL:HG23	2.20	0.41
1:B:2099:HIS:HB3	1:B:2102:ALA:HB2	2.01	0.41
1:A:473:THR:O	1:A:473:THR:HG22	2.20	0.41
1:A:608:MET:HE3	1:A:686:ILE:HG23	2.02	0.41
1:A:1363:ASP:O	1:A:1367:MET:HE2	2.20	0.41
1:A:1454:VAL:HG11	1:A:1465:TYR:HE2	1.85	0.41
1:A:1739:LEU:HD21	1:A:2224:PHE:CZ	2.56	0.41
1:A:2195:LEU:HD12	1:A:2195:LEU:N	2.35	0.41
1:B:1674:LEU:HA	1:B:1677:LEU:HD23	2.02	0.41
1:B:2198:LEU:O	1:B:2198:LEU:HD23	2.20	0.41
1:B:2239:LYS:HG2	1:B:2283:MET:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2260:PHE:HB2	1:B:2299:VAL:HG22	2.02	0.41
1:A:1318:GLU:O	1:A:1319:LYS:C	2.64	0.41
1:A:1469:ASP:O	1:A:1494:ALA:N	2.54	0.41
1:B:1120:ASP:HB2	1:B:2170:LEU:HD13	2.03	0.41
1:A:1878:SER:HB2	1:A:1941:ARG:HE	1.85	0.41
1:A:1960:LEU:CD1	1:A:2013:VAL:HG22	2.48	0.41
1:B:1403:MET:O	1:B:1403:MET:HE3	2.20	0.41
1:B:1474:THR:O	1:B:1478:MET:HG2	2.21	0.41
1:A:1360:GLU:H	1:A:1363:ASP:HB2	1.85	0.41
1:A:1940:LEU:HD13	1:A:2069:ILE:HD12	2.02	0.41
1:B:59:ASP:OD1	1:B:59:ASP:C	2.64	0.41
1:B:662:MET:SD	1:B:847:ALA:HB1	2.60	0.41
1:B:1655:ALA:O	1:B:1659:LEU:HD23	2.21	0.41
1:B:1824:ARG:O	1:B:1825:ARG:HD2	2.21	0.41
1:B:2096:THR:O	1:B:2100:ALA:N	2.53	0.41
1:A:788:LEU:HD12	1:A:831:LYS:HE2	2.03	0.41
1:A:952:TYR:CD2	1:A:954:GLU:HG2	2.56	0.41
1:A:1064:LEU:O	1:A:1065:ASP:HB3	2.20	0.41
1:A:2243:SER:OG	1:A:2283:MET:SD	2.79	0.41
1:B:759:LEU:HD13	1:B:766:ASN:ND2	2.26	0.41
1:B:1281:PHE:HZ	1:B:2335:VAL:HG22	1.86	0.41
1:B:1379:LEU:HG	1:B:1403:MET:HE1	2.03	0.41
1:B:1990:THR:HG22	1:B:1999:LEU:CD2	2.51	0.41
1:A:709:MET:HE1	1:A:775:TYR:HB2	2.02	0.40
1:B:834:LEU:O	1:B:834:LEU:HD23	2.21	0.40
1:B:967:PRO:O	1:B:969:HIS:N	2.55	0.40
1:B:1492:THR:HG21	1:B:1503:VAL:CG1	2.51	0.40
1:B:1568:ARG:O	1:B:1572:THR:HG23	2.21	0.40
1:B:2220:ASP:OD2	1:B:2222:LYS:NZ	2.54	0.40
1:A:640:PRO:HA	1:A:689:ALA:HB1	2.03	0.40
1:A:1499:GLY:HA2	1:A:1530:THR:HG21	2.04	0.40
1:A:1616:LEU:HD21	1:A:1624:ARG:HD2	2.03	0.40
1:A:1818:ASP:O	1:A:1822:ALA:N	2.48	0.40
1:A:2137:LEU:O	1:A:2142:GLY:HA3	2.21	0.40
1:B:111:MET:HE2	1:B:121:MET:HE2	2.03	0.40
1:B:1345:ARG:HA	1:B:1348:MET:HB3	2.03	0.40
1:B:1554:PRO:C	1:B:1558:MET:HE3	2.46	0.40
1:B:1688:LEU:C	1:B:1688:LEU:HD23	2.46	0.40
1:B:1963:GLU:N	1:B:1964:PRO:CD	2.85	0.40
1:A:1818:ASP:HA	1:A:1821:ASN:HB2	2.02	0.40
1:B:964:ARG:HH12	1:B:1027:ARG:CD	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1061:ARG:O	1:B:1061:ARG:HG2	2.22	0.40
1:A:932:LEU:C	1:A:932:LEU:HD23	2.45	0.40
1:A:1325:LEU:CD1	1:A:1351:ILE:HB	2.50	0.40
1:A:1640:LEU:HD12	1:A:1641:VAL:N	2.36	0.40
1:A:1723:THR:HG23	1:A:1733:HIS:HB3	2.02	0.40
1:A:2163:HIS:N	3:A:4102:NDP:O2X	2.47	0.40
1:A:2255:LEU:HD12	1:A:2255:LEU:N	2.36	0.40
1:A:2300:ILE:HG22	1:A:2359:LEU:HD12	2.03	0.40
1:B:822:ASP:OD1	1:B:823:LYS:N	2.54	0.40
1:B:1553:PHE:HB3	1:B:1554:PRO:HD3	2.04	0.40
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.97	0.40
1:A:957:LEU:HD11	1:A:978:ASP:HB3	2.02	0.40
1:A:1586:LEU:CD1	1:A:1611:VAL:HG11	2.51	0.40
1:A:1944:ILE:O	1:A:1948:VAL:HG23	2.21	0.40
1:B:564:PHE:N	1:B:564:PHE:CD2	2.89	0.40
1:B:630:SER:OG	1:B:632:LEU:HD23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	2376/4007 (59%)	2273 (96%)	103 (4%)	0	100	100
1	B	2376/4007 (59%)	2273 (96%)	103 (4%)	0	100	100
All	All	4752/8014 (59%)	4546 (96%)	206 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	1977/3338 (59%)	1963 (99%)	14 (1%)	76	77
1	B	1977/3338 (59%)	1955 (99%)	22 (1%)	65	73
All	All	3954/6676 (59%)	3918 (99%)	36 (1%)	68	75

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	279	ASP
1	A	603	VAL
1	A	960	ASN
1	A	1060	VAL
1	A	1119	LEU
1	A	1209	MET
1	A	1334	LEU
1	A	1355	VAL
1	A	1410	TRP
1	A	1794	ILE
1	A	1999	LEU
1	A	2019	MET
1	A	2339	ASP
1	B	47	GLU
1	B	152	MET
1	B	485	SER
1	B	557	THR
1	B	601	ILE
1	B	714	PHE
1	B	783	CYS
1	B	960	ASN
1	B	1052	ASP
1	B	1065	ASP
1	B	1066	SER
1	B	1133	MET
1	B	1313	ILE

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Mol	Chain	Res	Type
1	B	1325	LEU
1	B	1401	SER
1	B	1410	TRP
1	B	1478	MET
1	B	1500	ILE
1	B	2169	GLN
1	B	2217	MET
1	B	2240	VAL
1	B	2369	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	390	GLN
1	A	391	HIS
1	A	450	HIS
1	A	518	HIS
1	A	550	ASN
1	A	666	HIS
1	A	1070	HIS
1	A	1183	GLN
1	A	1665	HIS
1	A	1821	ASN
1	A	1967	HIS
1	A	2022	HIS
1	A	2143	GLN
1	A	2151	GLN
1	B	63	HIS
1	B	99	GLN
1	B	321	HIS
1	B	390	GLN
1	B	394	ASN
1	B	721	ASN
1	B	738	ASN
1	B	963	HIS
1	B	1032	GLN
1	B	1097	HIS
1	B	1256	ASN
1	B	1261	GLN
1	B	1322	HIS
1	B	1657	GLN

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Mol	Chain	Res	Type
1	B	1665	HIS
1	B	1670	ASN
1	B	1730	ASN
1	B	1945	GLN
1	B	2022	HIS
1	B	2233	GLN
1	B	2281	ASN
1	B	2377	HIS
1	B	2379	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NDP	B	4102	-	49,52,52	2.26	8 (16%)	66,80,80	1.63	12 (18%)
2	COZ	A	4101	-	44,50,50	0.91	1 (2%)	65,75,75	1.07	5 (7%)
2	COZ	B	4101	-	44,50,50	0.92	1 (2%)	65,75,75	1.12	5 (7%)
3	NDP	A	4102	-	49,52,52	2.27	8 (16%)	66,80,80	1.65	13 (19%)

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	NDP	B	4102	-	-	7/34/77/77	0/5/5/5
2	COZ	A	4101	-	-	15/48/64/64	0/3/3/3
2	COZ	B	4101	-	-	6/48/64/64	0/3/3/3
3	NDP	A	4102	-	-	14/34/77/77	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4102	NDP	P2B-O2B	12.53	1.83	1.59
3	B	4102	NDP	P2B-O2B	12.44	1.82	1.59
2	B	4101	COZ	P3B-O3B	5.01	1.68	1.59
2	A	4101	COZ	P3B-O3B	4.99	1.68	1.59
3	A	4102	NDP	PN-O5D	4.58	1.77	1.59
3	B	4102	NDP	PN-O5D	4.18	1.76	1.59
3	B	4102	NDP	O2B-C2B	-3.06	1.33	1.44
3	A	4102	NDP	O2B-C2B	-2.99	1.33	1.44
3	A	4102	NDP	C5A-C4A	2.59	1.43	1.39
3	B	4102	NDP	C5A-C4A	2.47	1.43	1.39
3	A	4102	NDP	C2A-N1A	2.28	1.38	1.33
3	B	4102	NDP	C2A-N1A	2.20	1.38	1.33
3	A	4102	NDP	C2B-C1B	2.13	1.58	1.53
3	A	4102	NDP	C8A-N9A	2.02	1.41	1.37
3	B	4102	NDP	C7N-N7N	2.02	1.38	1.33
3	A	4102	NDP	C7N-N7N	2.01	1.38	1.33
3	B	4102	NDP	C8A-N7A	2.00	1.35	1.31
3	B	4102	NDP	O5D-C5D	-2.00	1.37	1.44

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4102	NDP	PN-O3-PA	-7.13	108.36	132.83
3	B	4102	NDP	PN-O3-PA	-7.12	108.39	132.83
2	A	4101	COZ	C7P-N8P-C9P	3.44	128.72	122.59
3	B	4102	NDP	O2B-P2B-O1X	-3.39	96.32	109.39
2	B	4101	COZ	O6A-CCP-CBP	3.35	115.94	110.55
3	A	4102	NDP	O2B-P2B-O1X	-3.32	96.58	109.39
2	B	4101	COZ	C7P-N8P-C9P	3.18	128.26	122.59
3	A	4102	NDP	O4B-C4B-C3B	3.16	111.37	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4102	NDP	PN-O5D-C5D	-2.98	104.22	121.68
2	A	4101	COZ	C7P-C6P-C5P	-2.89	107.55	112.36
3	B	4102	NDP	PA-O5B-C5B	-2.89	104.76	121.68
3	A	4102	NDP	PA-O5B-C5B	-2.74	105.62	121.68
2	A	4101	COZ	O6A-CCP-CBP	2.61	114.74	110.55
3	A	4102	NDP	O3X-P2B-O2X	2.57	117.46	107.64
3	B	4102	NDP	O3X-P2B-O2X	2.53	117.32	107.64
3	A	4102	NDP	N3A-C4A-N9A	2.48	131.17	127.08
3	B	4102	NDP	N3A-C4A-N9A	2.38	131.00	127.08
3	A	4102	NDP	PN-O5D-C5D	-2.36	107.85	121.68
3	B	4102	NDP	C4B-O4B-C1B	-2.34	104.30	109.47
2	A	4101	COZ	CDP-CBP-CCP	-2.33	104.42	108.23
3	A	4102	NDP	C5A-C4A-N3A	-2.33	123.71	126.75
3	B	4102	NDP	C5A-C4A-N3A	-2.32	123.73	126.75
3	B	4102	NDP	O2N-PN-O1N	2.29	123.58	112.24
2	B	4101	COZ	C3B-C2B-C1B	2.28	104.95	99.89
3	A	4102	NDP	O5D-PN-O1N	-2.27	100.18	109.07
3	A	4102	NDP	C2A-N1A-C6A	-2.27	114.86	118.77
3	B	4102	NDP	C2A-N1A-C6A	-2.27	114.88	118.77
3	B	4102	NDP	C5B-C4B-C3B	-2.25	106.75	115.18
3	A	4102	NDP	O2N-PN-O1N	2.22	123.20	112.24
2	A	4101	COZ	CEP-CBP-CCP	2.18	111.79	108.23
3	B	4102	NDP	O5D-PN-O1N	-2.17	100.59	109.07
3	A	4102	NDP	C5B-C4B-C3B	-2.15	107.12	115.18
3	A	4102	NDP	C5D-C4D-C3D	-2.10	107.30	115.18
2	B	4101	COZ	CEP-CBP-CCP	2.09	111.64	108.23
2	B	4101	COZ	CDP-CBP-CCP	-2.01	104.95	108.23

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4101	COZ	CCP-O6A-P2A-O3A
2	A	4101	COZ	CCP-O6A-P2A-O4A
2	A	4101	COZ	C9P-CAP-CBP-CCP
2	A	4101	COZ	C9P-CAP-CBP-CDP
2	A	4101	COZ	C9P-CAP-CBP-CEP
2	A	4101	COZ	O9P-C9P-CAP-CBP
2	A	4101	COZ	N8P-C9P-CAP-CBP
2	A	4101	COZ	O9P-C9P-CAP-OAP
2	A	4101	COZ	N8P-C9P-CAP-OAP
2	B	4101	COZ	C5B-O5B-P1A-O1A

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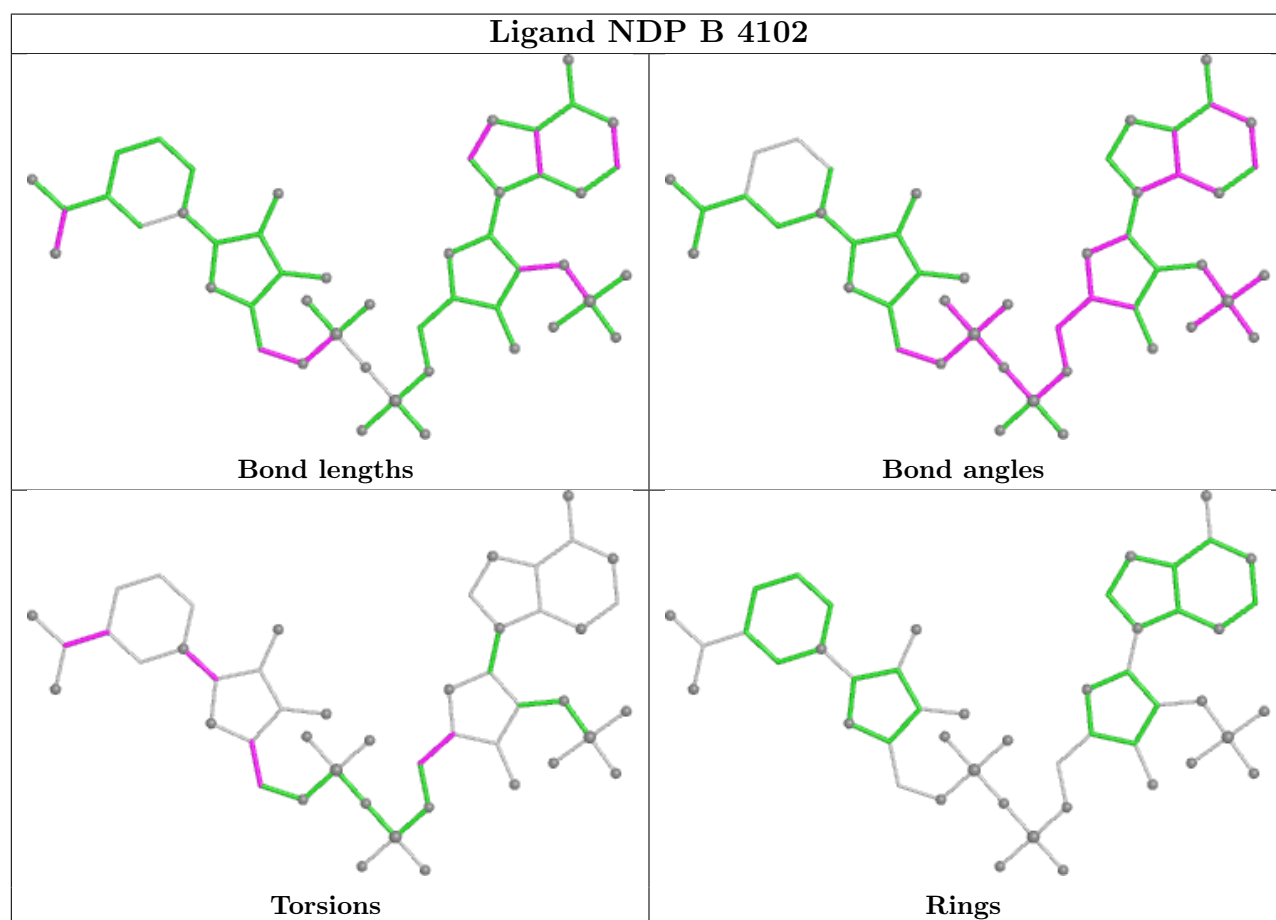
Mol	Chain	Res	Type	Atoms
2	B	4101	COZ	C5P-C6P-C7P-N8P
3	A	4102	NDP	C5B-O5B-PA-O1A
3	A	4102	NDP	C5B-O5B-PA-O2A
3	A	4102	NDP	C5D-O5D-PN-O1N
3	A	4102	NDP	C5D-O5D-PN-O2N
3	A	4102	NDP	O4D-C1D-N1N-C6N
3	A	4102	NDP	C2N-C3N-C7N-N7N
3	B	4102	NDP	C2D-C1D-N1N-C2N
3	B	4102	NDP	C2N-C3N-C7N-N7N
3	B	4102	NDP	C2D-C1D-N1N-C6N
3	A	4102	NDP	C4B-C5B-O5B-PA
2	A	4101	COZ	OAP-CAP-CBP-CDP
2	A	4101	COZ	OAP-CAP-CBP-CEP
2	B	4101	COZ	O4B-C4B-C5B-O5B
3	A	4102	NDP	O4D-C4D-C5D-O5D
2	A	4101	COZ	OAP-CAP-CBP-CCP
3	A	4102	NDP	C2N-C3N-C7N-O7N
3	B	4102	NDP	C2N-C3N-C7N-O7N
3	B	4102	NDP	O4D-C1D-N1N-C2N
2	B	4101	COZ	O4B-C1B-N9A-C8A
3	A	4102	NDP	O4B-C4B-C5B-O5B
3	B	4102	NDP	O4D-C4D-C5D-O5D
2	A	4101	COZ	C5B-O5B-P1A-O3A
2	B	4101	COZ	C5B-O5B-P1A-O3A
3	A	4102	NDP	C5B-O5B-PA-O3
3	A	4102	NDP	C5D-O5D-PN-O3
3	B	4102	NDP	O4B-C4B-C5B-O5B
3	A	4102	NDP	PA-O3-PN-O1N
3	A	4102	NDP	PA-O3-PN-O2N
2	A	4101	COZ	C5B-O5B-P1A-O2A
2	A	4101	COZ	O4B-C4B-C5B-O5B
2	B	4101	COZ	C9P-CAP-CBP-CCP

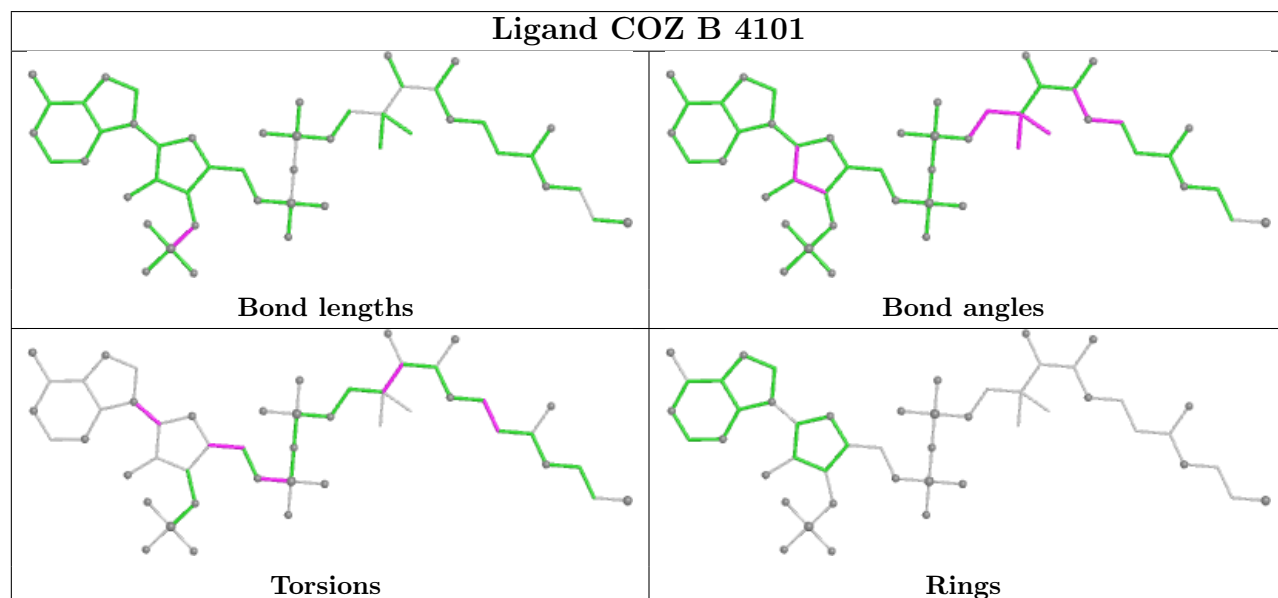
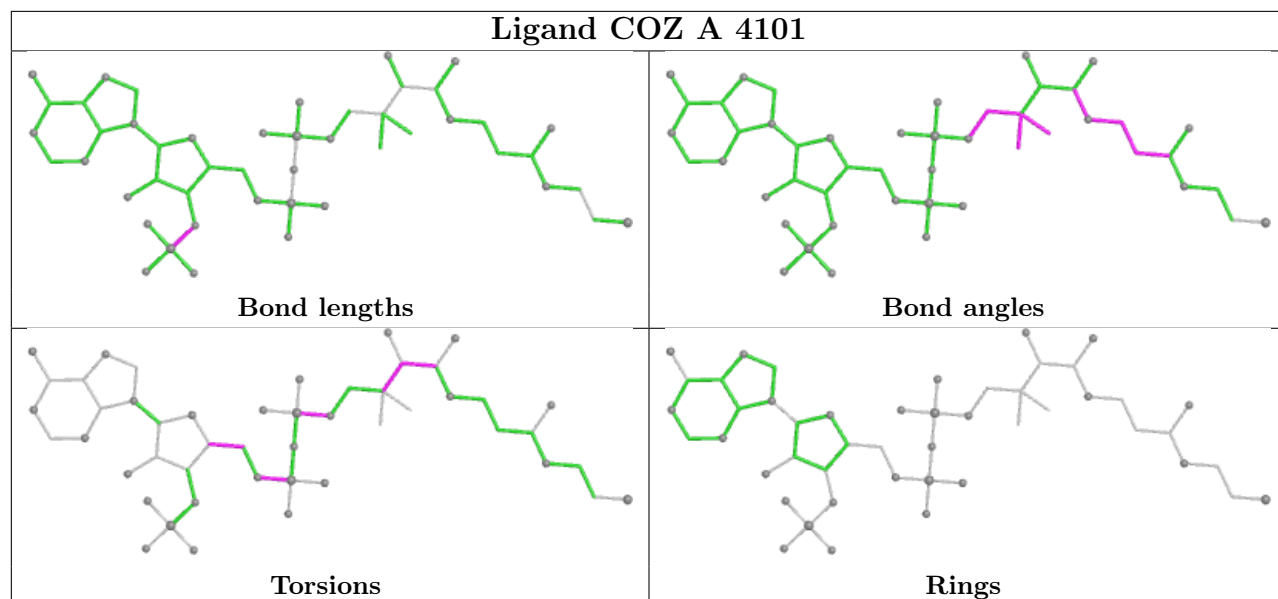
There are no ring outliers.

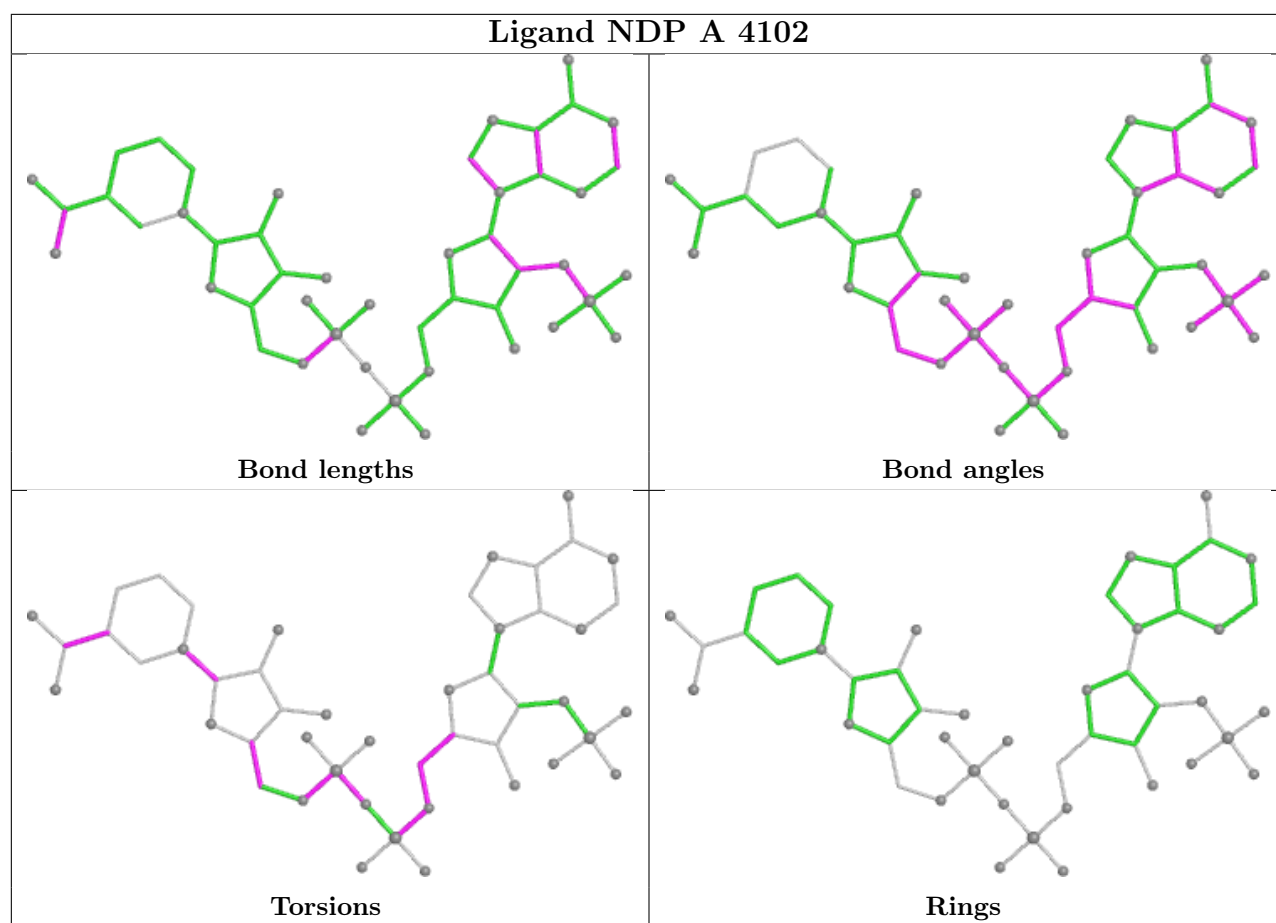
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4102	NDP	2	0
2	A	4101	COZ	2	0
2	B	4101	COZ	2	0
3	A	4102	NDP	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.